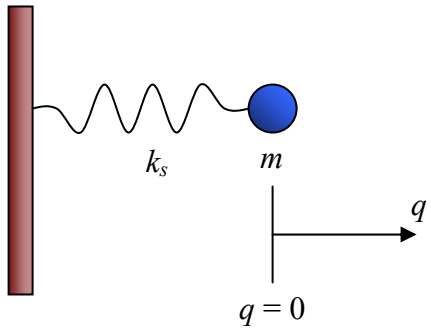
Harmonic Oscillations / Complex Numbers

Overview and Motivation: Probably the single most important problem in all of physics is the simple harmonic oscillator. It can be studied classically or quantum mechanically, with or without damping, and with or without a driving force. As we shall shortly see, an array of coupled oscillators is the physical basis of wave phenomena, the overarching subject of this course. In this lecture we will see how the differential equation that describes the simple harmonic oscillator naturally arises in a classical-mechanics setting. We will then look at several (equivalent) ways to write down the solutions to this differential equation.

Key Mathematics: We will gain some experience with the equation of motion of a classical harmonic oscillator, see a physics application of Taylor-series expansion, and review complex numbers.

I. Harmonic Oscillations

The freshman-physics concept of an (undamped, undriven) harmonic oscillator (HO) is something like the following picture, an object with mass m attached to an (immovable) wall with a spring with spring constant k_s. (There is no gravity here; only the spring provides any force on the object.)



Note that the oscillator has only two parameters, the **mass** m and **spring constant** k_s. Assuming that the mass is constrained to move in the horizontal direction, its **displacement** q (away from equilibrium) as a function of **time** t can be written as

$$q(t) = B\sin(\tilde{\omega}t + \phi), \tag{1}$$

where the **angular frequency** $\tilde{\omega}$ depends upon the oscillator parameters m and k_s via the relation $\tilde{\omega} = \sqrt{k_s/m}$. The **amplitude** B and the **phase** ϕ do not depend upon m and k_s, but rather depend upon the initial conditions (the initial displacement $q(0)$

and initial velocity $\frac{dq}{dt}(0)=\dot{q}(0)$ of the object). Note that the term **initial conditions** is a technical term that generally refers to the minimal specifications needed to describe the state of the system at time $t=0$. You should remember that the angular frequency is related to the (plain old) **frequency** ν via $\tilde{\omega}=2\pi\nu$ and that the frequency ν and **period** T are related via $\nu=1/T$.

Now because the sine and cosine functions are really the same function (but with just a shift in their argument by $\pm\pi/2$) we can also write Eq. (1) as

$$q(t)=B\cos(\tilde{\omega}t+\psi), \tag{2}$$

where the amplitude B is the same, but the phase $\psi=\phi-\pi/2$ (for the same initial conditions). It probably is not obvious (yet), but we can also write Eq. (1) as

$$q(t)=D\cos(\tilde{\omega}t)+E\sin(\tilde{\omega}t), \tag{3}$$

where the amplitudes D and E depend upon the initial conditions of the oscillator. Note that the term **harmonic function** simply means a sine or cosine function. Note also that all three forms of the displacement each have two parameters that depend upon the initial conditions.

II. Classical Origin of Harmonic Oscillations

A. The Harmonic Potential

The harmonic motion of the classical oscillator illustrated above comes about because of the nature of the spring force (which is the only force and thus the net force) on the mass, which can be written as

$$F_s(q)=-k_s q. \tag{4}$$

Because the spring force is conservative, F_s can be derived from a **potential energy function** $V(q)$ via the general (in 1D) relationship

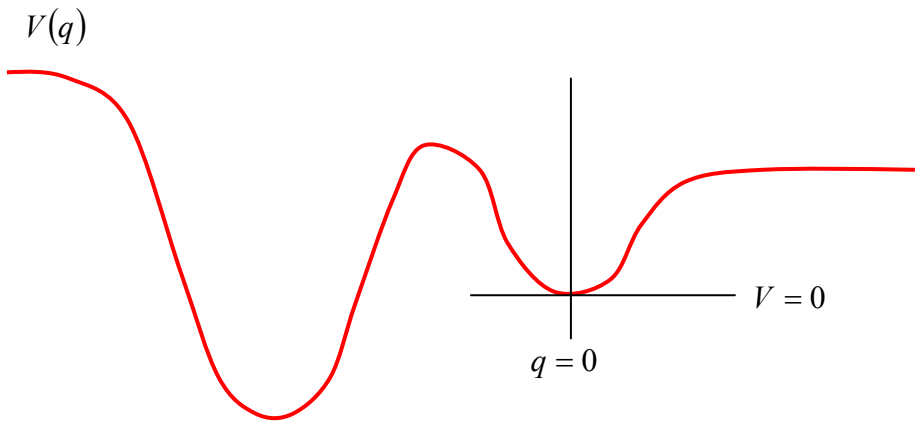
$$F(q)=-\frac{dV(q)}{dq}. \tag{5}$$

A potential energy function for the spring that gives rise to Eq. (4) for the spring force is

$$V_s(q) = \frac{1}{2} k_s q^2 \tag{6}$$

(do the math!).

Let's see how the potential energy represented by Eq. (6) arises in a rather general way. Let's consider an object constrained to move in one dimension (like the oscillator above). However, in this case all we know is that the potential energy function has at least one local minimum, as illustrated in the following graph of $V(q)$ vs q.



Let's now assume that the mass is located near the potential energy minimum on the right side of the graph and that its energy is such that it does not move very far away from this minimum. Just because we can, let's also assume that this minimum defines where $q = 0$ and $V = 0$, as shown in the picture.

Now here is where some math comes in. If the mass does not move very far away from $q = 0$ then we are only interested in motion for small q. Let's see what the potential energy function looks like in this case. For small q it makes sense to expand the function $V(q)$ in a **Taylor series**

$$V(q) = V(0) + V'(0)q + \frac{1}{2}V''(0)q^2 + \frac{1}{6}V'''(0)q^3 + \ldots, \tag{7}$$

where, e.g., $V'(0)$ is the first derivative of V evaluated at $q = 0$. Now the rhs of Eq. (7) has an infinite number of terms and so is generally quite complicated, but often only one of these terms is important. Let's look at each term in order. The first term $V(0)$ is zero because we defined the potential energy at this minimum to be zero. So far so good. The next term is also zero because the slope of the function $V(q)$ is also zero at

the minimum. The next term is not zero and neither, in general, are any of the others. However, if q is small enough, these other terms are negligible compared to the third (quadratic) term.[1] Thus, if the object's motion is sufficiently close to the minimum in potential energy, then we have

$$V(q) \approx \frac{1}{2} V''(0) q^2 . \tag{8}$$

So this is pretty cool. Even though we have no idea what the potential energy function is like, except that it has a minimum somewhere, we see that if the object is moving sufficiently close to that minimum, then the potential energy is the same as for a mass attached to a spring where the effective spring constant k_s is simply the curvature V'' evaluated at the potential energy minimum ($q = 0$), $V''(0)$.[2] Equation (8) is known as the **harmonic approximation** to the potential $V(q)$ (near the minimum).

B. Harmonic Oscillator Equation of Motion

OK, so we see that the potential energy near a minimum is equivalent to the potential energy of an harmonic oscillator. If we happen to know how an harmonic oscillator behaves, then we know how our mass will behave near the minimum. But let's assume for the moment that we know nothing about the specifics of a harmonic oscillator. Where do we go from here to determine the motion of the mass near the minimum? Well, as in most classical mechanics problems we use **Newton's second law**, which is generally written (for 1D motion) as

$$a = \frac{F_{net}}{m} , \tag{9}$$

where a is the acceleration of the object and F_{net} is the **net force** (i.e., sum of all the forces) on the object.

In the case at hand, in which the object's acceleration is $d^2q/dt^2 = \ddot{q}$ and the net force comes only from the potential energy (near the minimum) Eq. (9) becomes

[1] In physics we are often interested in comparing terms in expressions such as Eq. (7), and we often use the comparators >> and << to compare these terms. These two comparators actually mean $< \frac{1}{10}\times$ and $> 10\times$, respectively. For example, $a >> b$ indicates that $a > 10b$.

[2] Exceptions can occur. If the potential minimum is so flat that $V''(0) = 0$ then the third term will be zero and it will be some higher-order term(s) that determine(s) the motion near the potential-energy minimum. The object will oscillate, but it will not oscillate harmonically.

$$\ddot{q} = -\frac{V''(0)}{m} q \,, \tag{10}$$

or, identifying $V''(0)$ as the spring constant k_s we can write Eq. (10) as

$$\ddot{q} + \frac{k_s}{m} q = 0 \,. \tag{11}$$

Equation (11) is known as the **equation of motion** for an harmonic oscillator. Generally, the equation of motion for an object is the specific application of Newton's second law to that object. Also quite generally, the classical equation of motion is a differential equation such as Eq. (11). As we shall shortly see, Eq. (11) along with the initial conditions $q(0)$ and $\dot{q}(0)$ completely specify the motion of the object near the potential energy minimum. Note that two initial conditions are needed because Eq. (11) is a second-order equation.

Let's take few seconds to classify this differential equation. It is **second order** because the highest derivative is second order. It is **ordinary** because the derivatives are only with respect to one variable (t). It is **homogeneous** because q or its derivatives appear in every term, and it is **linear** because q and its derivatives appear separately and linearly in each term (where they appear). An major consequence of the homogeneity and linearity is that linear combinations of solutions to Eq. (11) are also solutions. This fact will be utilized extensively throughout this course.

C. HO Initial Value Problem

The solution to Eq. (11) can be written most generally as either Eq. (1), Eq. (2), or Eq. (3) (where $\tilde{\omega} = \sqrt{k_s/m}$). Let's consider Eq. (3)

$$q(t) = D\cos(\tilde{\omega}t) + E\sin(\tilde{\omega}t), \tag{3}$$

and see that indeed the constants D and E are determined by the initial conditions. By applying the initial conditions we are solving the **initial value problem** (IVP) for the HO. Setting $t = 0$ in Eq. (3) we have

$$q(0) = D \tag{12}$$

Similarly, taking the time derivative of Eq. (3)

$$\dot{q}(t) = -\tilde{\omega}D\sin(\tilde{\omega}t) + \tilde{\omega}E\cos(\tilde{\omega}t) \tag{13}$$

and again setting $t = 0$ gives us

$$\dot{q}(0) = \tilde{\omega}E \,. \tag{14}$$

Hence, the general solution to the (undamped, undriven) harmonic oscillator problem can be written as

$$q(t) = q(0)\cos(\tilde{\omega}t) + \frac{\dot{q}(0)}{\tilde{\omega}}\sin(\tilde{\omega}t). \tag{15}$$

To summarize, for a given set of initial conditions $q(0)$ and $\dot{q}(0)$, Eq. (15) is the solution to Eq. (11), the harmonic oscillator equation of motion.

III. Complex Numbers

In our discussion so far, all quantities are real number (with possibly some units, such as $q = 3$ cm). However, when dealing with harmonic oscillators and wave phenomena, it is often useful to make use of complex numbers, so let's briefly review some facts regarding complex numbers.

The key definition associated with complex numbers is the square root of -1, known as i. That is, $i = \sqrt{-1}$. From this all else follows.

Any complex number z can always be represented in the form

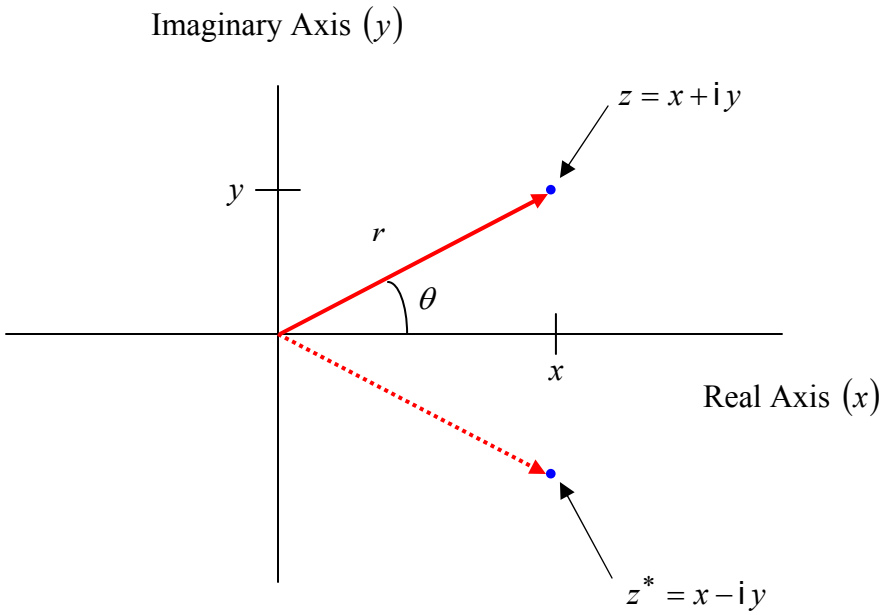
$$z = x + iy \,, \tag{16}$$

where x and y are both *real* numbers. Common notations for the real and imaginary parts of z are $x = \mathrm{Re}(z)$ and $y = \mathrm{Im}(z)$. It is also often convenient to represent a complex number as a point in the complex plane, in which the x coordinate is the real part of z and the y coordinate is the imaginary part of z, as illustrated by the picture on the following page.

As this can be inferred from this picture, we can also use polar coordinates r and θ to represent a complex number as

$$z = r\cos(\theta) + ir\sin(\theta) = r[\cos(\theta) + i\sin(\theta)]. \tag{17}$$

Using the infamous **Euler relation** (which you should never forget!)



$$e^{i\theta} = \cos(\theta) + i\sin(\theta) \tag{18}$$

we see that a complex number can also be written as

$$z = re^{i\theta}\,. \tag{19}$$

The last important definition associated with complex numbers is the complex conjugate of z defined as

$$z^* = x - iy\,. \tag{20}$$

As is apparent in the diagram above, this amounts to a reflection about the real (x) axis. Note the following relationships:

$$\frac{z + z^*}{2} = x = \mathrm{Re}(z), \tag{21}$$

$$\frac{z - z^*}{2i} = y = \mathrm{Im}(z),$$

and

$$zz^* = x^2 + y^2 = r^2 . \tag{22}$$

Note also the absolute value of a complex number, which is equal to r, is given by

$$|z| = r = \sqrt{zz^*} . \tag{23}$$

IV. Complex Representations of Harmonic Oscillator Solutions

Because the HO equation of motion [Eq. (11)] is linear and homogeneous, linear combinations of solutions are also solutions. These linear combinations can be complex combinations. For example, because $\cos(\tilde{\omega}t)$ and $\sin(\tilde{\omega}t)$ are both solutions to Eq. (11) (we are not worrying about any particular initial conditions at the moment), another solution to Eq. (11) is the complex linear combination

$$q(t) = \alpha\cos(\tilde{\omega}t) + i\alpha\sin(\tilde{\omega}t) = \alpha e^{i\tilde{\omega}t} , \tag{24}$$

where α is some complex number.

So what is the point here? Well, as we shall see as we go along, it is often convenient to work with complex representations of solutions to the harmonic oscillator equation of motion (or to the wave equation that we will be dealing with later). So what does it mean to have a complex displacement? Nothing, really – a displacement cannot be complex, it is indeed a real quantity. So if we are dealing with a complex solution, what do we do to get a physical (real) answer? There are at least three approaches:

(1) The first approach is to, up front, make the solution manifestly real. For example, let's say you want to work with the general complex solution

$$q(t) = \alpha e^{i\tilde{\omega}t} + \beta e^{-i\tilde{\omega}t} , \tag{25}$$

where α and β are complex numbers. You can impose the condition $\beta = \alpha^*$, which results in $q(t)$ being real.

(2) Another approach is to simply work with the complex solution until you need to doing something such as impose the initial conditions. Then, for example, if we are working with the form in Eq. (25), the initial conditions might be something like $\mathrm{Re}[q(0)] = A$, $\mathrm{Im}[q(0)] = 0$, $\mathrm{Re}[\dot{q}(0)] = B$, and $\mathrm{Im}[\dot{q}(0)] = 0$. These four conditions would then determine the four unknowns, the real and imaginary parts of α and β (and again would result in $q(t)$ being real).

(3) A third approach is to simply use the real part of a solution when something like the initial conditions are needed, and then impose the initial conditions. (Alternatively, because the imaginary part of the solution is also a real number, you could use the imaginary part of the solution if you were so inclined.)

Note that these different approaches work because the harmonic oscillator equation of motion is real and linear. We will not worry about the details of this at the moment, but if you are interested you can read more about this on pp. 9-10 of Dr. Torre's text, *Foundations of Wave Phenomena* (FWP).

Exercises

*__2.1__ Show that Eqs. (1) and (2) are solutions to Eq. (11), the equation of motion for the harmonic oscillator.

*__2.2__ Assuming the form of Eq. (1) for the solution to Eq. (11), find the values of B and ϕ in terms of the initial conditions $q(0)$ and $\dot{q}(0)$.

*__2.3__ Assuming the form of Eq. (2) for the solution to Eq. (11), find the values of B and ψ in terms of the initial conditions $q(0)$ and $\dot{q}(0)$. [This exercise along with Exercise 2.2 shows that Eqs. (1) and (2) are equivalent.]

**__2.4 Quadratic approximation to a particular potential energy__. Consider the potential energy function $V(q)=1-\cos(\kappa q)$, where κ is some positive constant.
(a) Carefully (!) plot (using a computer math program such as Mathcad, Maple, etc.) this function for $-\pi<\kappa q<\pi$ (For simplicity in making this and the following graph you may set κ to 1) **Make sure that your axes are carefully labeled on this and all other graphs**.
(b) Find the force $F(q)$ associated with this potential-energy function (for arbitrary positive κ).
(c) Taylor series expand the potential-energy function about the point $q=0$; keep all terms up to the q^4 term.
(d) What is the effective spring constant k_s associated with this potential-energy function?
(e) What condition on $|q|$ is necessary so that the q^4 term (in the Taylor series expansion) is much smaller (<<) that the (harmonic) q^2 term? (See footnote 1 on p. 4.)
(f) Replot the original function $V(q)=1-\cos(\kappa q)$ and the **harmonic** approximation to this function from $-\pi<\kappa q<\pi$. Based on this graph, for what values of κq do you expect the harmonic approximation to be valid? How does this compare to your answer in (e)?

2.5 **The Euler relation. The Euler relation $e^{i\theta} = \cos(\theta) + i\sin(\theta)$ can be shown to be true by comparing, term by term, the Taylor series of both sides of the relation. Calculate the first five Taylor series terms (about $\theta = 0$, so these will be the θ^0, θ^1, θ^2, θ^3, θ^4, and θ^5 terms) of each side of the equation and show that they are equivalent.

*2.6 Write the following complex expressions in the form $x + iy$

(a) $5e^{i(\pi/4)}$

(b) $(5-4i)(3+2i)$

(c) $\dfrac{1}{6-7i}$

(d) $2e^{i\pi} \cdot 16e^{-i(\pi/2)}$

*2.7 Write the expressions in Exercise 2.6 in the form $Ae^{i\theta}$, where A and θ are both real.

*2.8 Find the real part of $q(t) = \alpha e^{i\tilde{\omega}t} + \alpha^* e^{-i\tilde{\omega}t}$. Here α is complex. Write your solution in terms of $\mathrm{Re}(\alpha)$, $\mathrm{Im}(\alpha)$, $\sin(\tilde{\omega}t)$, and $\cos(\tilde{\omega}t)$.

*2.9 **Complex solution and initial conditions**

(a) Show that $q(t) = \alpha e^{i\tilde{\omega}t} + \beta e^{-i\tilde{\omega}t}$ is a solution to Eq. (11), the harmonic oscillator equation of motion.

(b) Assuming that α and β are complex, find α and β in terms of the initial conditions $q(0)$ and $\dot{q}(0)$. (Do this using one of the three methods discussed on p. 8.)

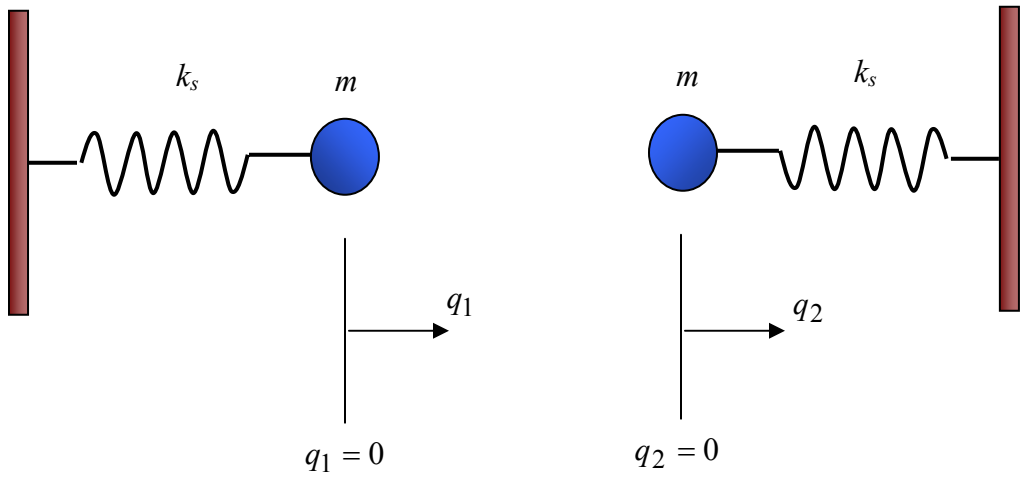
Two Coupled Oscillators / Normal Modes

Overview and Motivation: Today we take a small, but significant, step towards wave motion. We will not yet observe waves, but this step is important in its own right. The step is the coupling together of two oscillators via a spring that is attached to both oscillating objects.

Key Mathematics: We gain some experience with coupled, linear ordinary differential equations. In particular we find special solutions to these equations, known as normal modes, by solving an eigenvalue problem.

I. Two Coupled Oscillators

Let's consider the diagram shown below, which is nothing more than 2 copies of an harmonic oscillator, the system that we discussed last time. We assume that both oscillators have the same mass m and spring constant k_s. Notice, however, that because there are two oscillators each has it own displacement, either q_1 or q_2.



Based on the discussion last time you should be able to immediately write down the equations of motion (one for each oscillating object) as

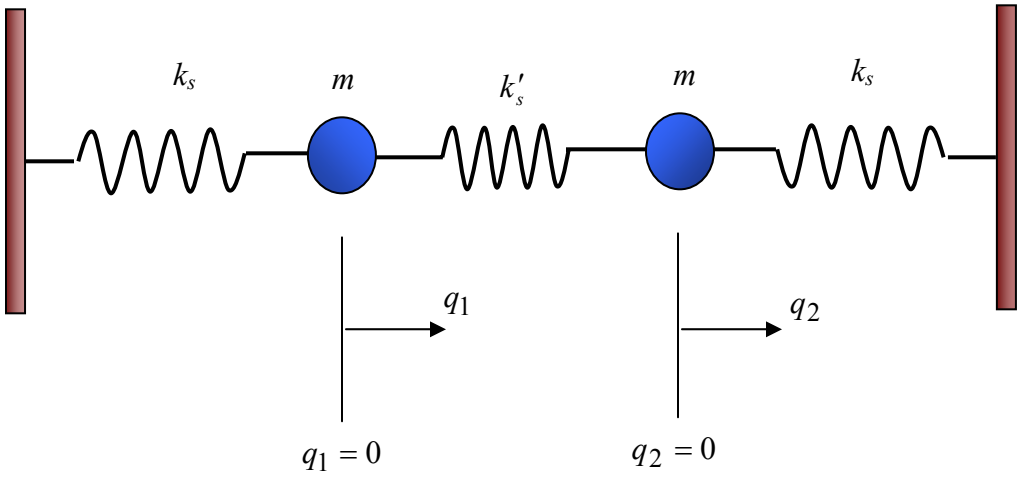
$$\ddot{q}_1 + \tilde{\omega}^2 q_1 = 0, \text{ and} \tag{1a}$$

$$\ddot{q}_2 + \tilde{\omega}^2 q_2 = 0, \tag{1b}$$

where $\tilde{\omega}^2 = k_s/m$. As we saw last time, the solution to each of theses equations is harmonic motion at the (angular) frequency $\tilde{\omega}$. As should be obvious from the

picture, the motion of each oscillator is independent of the other oscillator. This is also reflected in the equation of motion for each oscillator, which has nothing to do with the other oscillator.

Let's now make things a bit more interesting by adding in another spring that connects the two oscillating objects together, as illustrated in the following picture. To make things even more interesting we assume that this new spring has a different constant k_s'. However, to keep things simple we assume that the middle spring provides no force if $q_1 - q_2 = 0$. That is, this spring is neither stretched or compressed if its length is equal to the its length when two objects are at equilibrium.



Thinking about this picture we should realize that the two equations of motion will no longer be independent. That is, the equation of motion for the first object will depend (somehow) upon what the second object is doing, and vice versa.

Let's use Newton's second law to write down the equation motion for each object. Recall that Newton's second law for either object ($i = 1,2$) can be written as

$$\ddot{q}_i = \frac{F_i}{m}, \tag{2}$$

where F_i is the net force on object i. The tricky part, if there is a tricky part, is to determine the sum F_i on each object. The net force on the first object comes from the spring on the left and the spring in the middle. With a little thought you should realize that this net force F_1 is

$$F_1 = -k_s q_1 - k_s'(q_1 - q_2). \tag{3a}$$

Make sure that you understand the signs of all the term on the rhs of this equation. Notice that the force provided by the middle spring depends not only on the first object's displacement but also on the second object's displacement. Similarly, the net force on the second object is

$$F_2 = -k_s q_2 - k_s'(q_2 - q_1). \tag{3b}$$

Substituting these two forces into Eq. (2), once for each object, we obtain the two equations of motion,

$$\ddot{q}_1 + \tilde{\omega}^2 q_1 + \tilde{\omega}'^2(q_1 - q_2) = 0 \tag{4a}$$

for the first object and

$$\ddot{q}_2 + \tilde{\omega}^2 q_2 + \tilde{\omega}'^2(q_2 - q_1) = 0 \tag{4b}$$

for the second. Here $\tilde{\omega}'^2 = k'/m$. Given the symmetry of the problem, it might not surprise you that you can obtain one equation of motion from the other with the transformation $1 \leftrightarrow 2$ in the subscripts that label the objects.

So now we have a considerably more complicated problem: as expected from looking at the drawing above, the equation of motion for each object depends upon what the other object is doing. Specifically, each equation of motion depends upon the displacement of the other object.

II. Normal Modes

A. Harmonic Ansatz

So what are the solutions to these differential equations? Well, we will eventually write down the general solution (next lecture). But right now we are going to look at a special class of solutions known as normal-mode solutions, or simply, normal modes. A **normal mode** is a solution in which both masses harmonically oscillate at the same frequency. We state why these special solutions are extremely useful at the end of the lecture. For now let's see if we can find them. We use the complex form of harmonic motion and write

$$q_1(t) = q_{01} e^{i\Omega t} \text{ and} \tag{5a}$$

$$q_2(t) = q_{02}e^{i\Omega t}\,. \tag{5b}$$

Notice that the (unknown) **frequency of oscillation** Ω of both oscillators is the same, a key feature of a normal mode. Also, because we are using the complex form of harmonic motion, the amplitudes q_{01} and q_{02} may be complex, but they too are unknown at this point. Keep in mind that Eq. (5) is only the form of a normal-mode solution: it is only a solution if it satisfies the equations of motion. In other words, we now need to find values of the frequency Ω and amplitudes q_{01} and q_{02} that satisfy Eqs. (4a) and (4b), the equations of motion.

So let's substitute Eq. (5) into Eq. (4) and see what that tells us about Ω, q_{01}, and q_{02}. Carrying out the substitution and calculating the derivatives yields

$$-\Omega^2 q_{01}e^{i\Omega t} + \tilde{\omega}^2 q_{01}e^{i\Omega t} + \tilde{\omega}'^2\left(q_{01}e^{i\Omega t} - q_{02}e^{i\Omega t}\right) = 0\,, \text{ and} \tag{6a}$$

$$-\Omega^2 q_{02}e^{i\Omega t} + \tilde{\omega}^2 q_{02}e^{i\Omega t} + \tilde{\omega}'^2\left(q_{02}e^{i\Omega t} - q_{01}e^{i\Omega t}\right) = 0\,. \tag{6b}$$

Dividing by $e^{i\Omega t}$ (Is this legal?) and rearranging some terms gives

$$\left(\tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2\right)q_{01} - \tilde{\omega}'^2 q_{02} = 0\,, \text{ and} \tag{7a}$$

$$-\tilde{\omega}'^2 q_{01} + \left(\tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2\right)q_{02} = 0\,. \tag{7b}$$

So what do we have here? We have two algebraic equations and three unknowns Ω, q_{01}, and q_{02}. The problem seems a bit underspecified, and it is: as we shall see below, we will only be able to solve for Ω and the ratio q_{01}/q_{02}.

B. Eigenvalue Problem

If you have previously studied differential equations and linear algebra you may be inclined to write Eq. (7) in matrix notation as

$$\begin{pmatrix} \tilde{\omega}^2 + \tilde{\omega}'^2 & -\tilde{\omega}'^2 \\ -\tilde{\omega}'^2 & \tilde{\omega}^2 + \tilde{\omega}'^2 \end{pmatrix}\begin{pmatrix} q_{01} \\ q_{02} \end{pmatrix} = \Omega^2\begin{pmatrix} q_{01} \\ q_{02} \end{pmatrix}, \tag{8}$$

which you would recognize as an **eigenvalue problem**. Generally, an eigenvalue problem is one where some **linear operator** (in this case a matrix) operating on some object (in this case a 2D column **vector**) produces a constant (in this case Ω^2) times the original object. Generally, an N-dimensional linear-algebra eigenvalue problem

has N solutions [which consist of special values of the constant (or **eigenvalue**) Ω^2 and amplitudes $q_{01}\ldots q_{0n}$ (or **eigenvector** $\begin{pmatrix} q_{01} \\ \vdots \\ q_{0N} \end{pmatrix}$)].

C. Eigenvalues

Well, that was a lot of terminology, but what about the solution? Well, let's rewrite Eq. (8) as

$$\begin{pmatrix} \tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2 & -\tilde{\omega}'^2 \\ -\tilde{\omega}'^2 & \tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2 \end{pmatrix} \begin{pmatrix} q_{01} \\ q_{02} \end{pmatrix} = 0 . \tag{9}$$

Now this is interesting. Expressed in this way, we have the product of two quantities equal to zero. There are two ways that Eq. (9) can be true. The first, which is the trivial (i.e., uninteresting) solution, is $q_{01} = q_{02} = 0$. Physically, this corresponds to no motion of the system – pretty uninteresting! The nontrivial way that Eq. (9) can be satisfied is if the **determinant** of the 2 × 2 matrix is zero. That is

$$\begin{vmatrix} \tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2 & -\tilde{\omega}'^2 \\ -\tilde{\omega}'^2 & \tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2 \end{vmatrix} = 0 . \tag{10}$$

For a 2×2 matrix the determinant is easily calculated, $\begin{vmatrix} A & B \\ C & D \end{vmatrix} = AD - BC$, so in this case Eq. (10) can be expressed as

$$\left(\tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2\right)^2 - \tilde{\omega}'^4 = 0 . \tag{11}$$

Eq. (11) [or Eq. (10)] is known as the **characteristic equation** for the eigenvalue problem. This is great! We now have an equation for the eigenvalue Ω^2 and thus the normal-mode frequency Ω,

$$\tilde{\omega}^2 + \tilde{\omega}'^2 - \Omega^2 = \pm\tilde{\omega}'^2 . \tag{12}$$

Solving Eq. (12) for Ω^2 produces the two eigenvalues

$$\Omega^2 = \tilde{\omega}^2, \tilde{\omega}^2 + 2\tilde{\omega}'^2 , \tag{13}$$

which gives us four solutions for the normal-mode frequency

$$\Omega = \pm\tilde{\omega}, \pm\sqrt{\tilde{\omega}^2 + 2\tilde{\omega}'^2}\ . \tag{14}$$

D. Eigenvectors and Normal Modes

So now that we have the eigenvalues $\tilde{\omega}^2$ and $\tilde{\omega}^2 + 2\tilde{\omega}'^2$, we need to find the eigenvector associated with each eigenvalue. To do this we substitute each eigenvalue into either Eq. (7a) or (7b) (It doesn't matter which, you get the same equation in either case).

1. first normal mode

For the first eigenvalue, $\Omega^2 = \tilde{\omega}^2$, this substitution produces

$$\tilde{\omega}'^2 q_{01} - \tilde{\omega}'^2 q_{02} = 0, \tag{15}$$

which gives us the result for the amplitudes

$$q_{01} = q_{02}, \tag{16}$$

and so the eigenvector associated with the first normal mode is $\begin{pmatrix}1\\1\end{pmatrix}$. This result tells us that both oscillators oscillate identically [check out Eq. (5) with the result of Eq. (16)] if this normal mode is excited. That is, the objects oscillate with exactly the same amplitude and the same phase.

Now because the eigenvalue $\Omega^2 = \tilde{\omega}^2$ corresponds to two normal-mode frequencies $\Omega = \pm\tilde{\omega}$, this first eigensolution of the linear algebra problem gives us to two linearly-independent solutions to the equations of motion.

$$q_1(t) = A_1 e^{i\tilde{\omega}t} \text{ and } q_2(t) = A_1 e^{i\tilde{\omega}t} \tag{17a),(17b}$$

is the first solution, and

$$q_1(t) = B_1 e^{-i\tilde{\omega}t} \text{ and } q_2(t) = B_1 e^{-i\tilde{\omega}t} \tag{18a),(18b}$$

is the second, where the amplitudes A_1 and B_1 are arbitrary. Equations (17) and (18) can be written in linear-algebra inspired notation as

$$\begin{pmatrix}q_1(t)\\q_2(t)\end{pmatrix}_{1+} = A_1\begin{pmatrix}1\\1\end{pmatrix}e^{i\tilde{\omega}t} \tag{19}$$

and

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{1-} = B_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-i\tilde{\omega}t}, \tag{20}$$

respectively. The $1+$ and $1-$ denote the $+\tilde{\omega}$ and $-\tilde{\omega}$ solutions. However, because oscillations at frequency $-\tilde{\omega}$ are really just oscillations at $\tilde{\omega}$, any linear combination of these two solutions really just oscillates at the frequency $\tilde{\omega}$, and so any linear combination of Eq. (19) and (20) can be thought of as the first normal-mode solution at frequency $\tilde{\omega}$. That is, the most general way we can write the first normal-mode solution is

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_1 = \begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{1+} + \begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{1-} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \left(A_1 e^{i\tilde{\omega}t} + B_1 e^{-i\tilde{\omega}t} \right), \tag{21}$$

where A_1 and B_1 are unspecified constants. Note that arbitrariness of A_1 and B_1 is consistent with our knowledge that for an harmonic oscillator the frequency is independent of the amplitude. Note also that (if we wish to at this point) we can specify the solution to be real, in which case we would set $B_1 = A_1^*$.

2. second normal mode

Let's now look at the second normal-mode solution, which corresponds to the second eigenvalue $\tilde{\omega}^2 + 2\tilde{\omega}'^2$. As before, we substitute this eigenvalue into Eq. (7a), which gives us

$$-\tilde{\omega}'^2 q_{01} - \tilde{\omega}'^2 q_{02} = 0 \tag{22}$$

or

$$q_{01} = -q_{02}, \tag{23}$$

and so the eigenvector associated with the second normal mode is $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. So if this normal mode is excited the two oscillators oscillate with the same amplitude, but with opposite phase (or a phase difference of $\pi/2$). That is, when the first oscillator is moving to the left the second is moving to the right with the same magnitude in its displacement, and vice versa.

As in the case of the first eigenvalue, there are two linearly-independent solutions corresponding to the two frequencies $\pm\sqrt{\tilde{\omega}^2 + 2\tilde{\omega}'^2}$. The first solution is

$$q_2(t) = A_2 e^{i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t} \text{ and } q_2(t) = -A_2 e^{i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t} \qquad \text{(24a),(24b)}$$

and the second is

$$q_1(t) = B_2 e^{-i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t} \text{ and } q_2(t) = -B_2 e^{-i\sqrt{\omega^2+2\omega'^2}\,t}, \qquad \text{(25a),(25b)}$$

or in linear-algebra notation

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{2-} = A_2 \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t} \qquad (26)$$

and

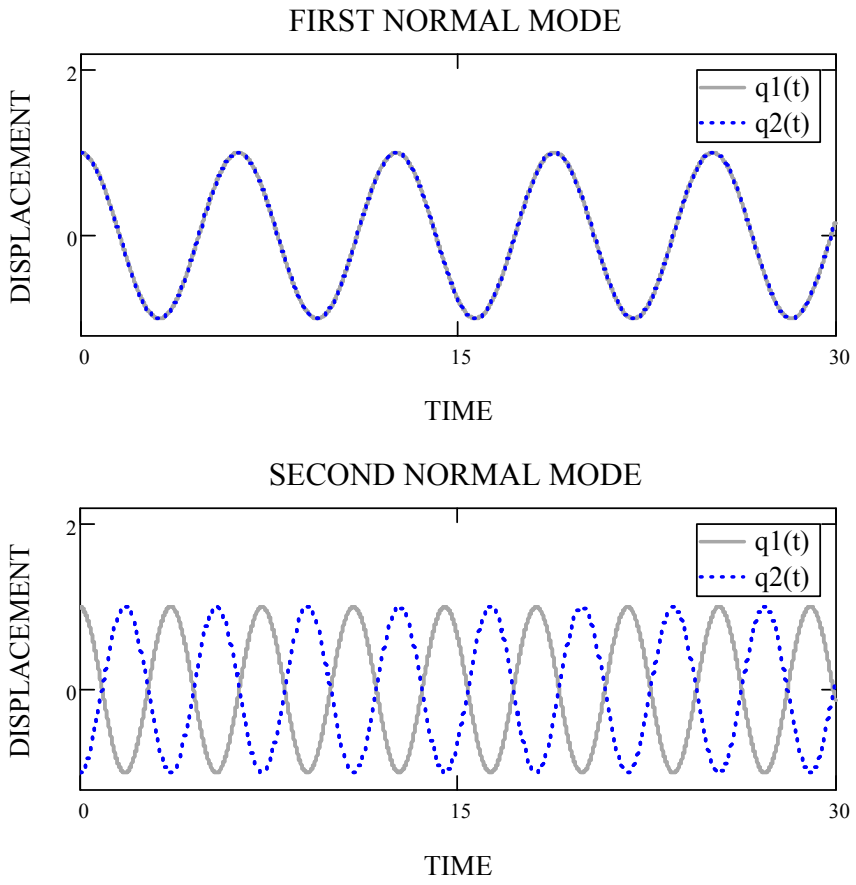
$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{2-} = B_2 \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{-i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t}. \qquad (27)$$

As before, the general form of this normal-mode solution is

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{2} = \begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{2+} + \begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_{2-} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \left(A_2 e^{i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t} + B_2 e^{-i\sqrt{\tilde{\omega}^2+2\tilde{\omega}'^2}\,t} \right) \qquad (28)$$

The graphs on the following page plot the time-dependent amplitudes $q_1(t)$ and $q_2(t)$ for the two normal modes for the following values of the arbitrary constants: $A_1 = B_1 = 1/2$ for the first normal mode and $A_2 = B_2 = 1/2$ for the second normal mode. (With these choices the solutions are real.) For these graphs we have also set m, k_s, and k_s' equal to 1, so that $\tilde{\omega} = 1$ and $\sqrt{\tilde{\omega}^2 + 2\tilde{\omega}'^2} = \sqrt{3}$. (Admittedly, we have not specified units here, but if standard SI units are used for the mass, spring constants, and time, then the unit for displacement is meters.) As the graphs show, in the first normal mode the two objects oscillate identically, while in the second normal mode they oscillate exactly oppositely.

As we will see in the next lecture, a great usefulness of the normal mode solutions is that ANY solution of Eqs. (4a) and (4b), the equations of motion for this coupled oscillator system, can be written as a linear combination of these two normal-mode solutions. Indeed, this property of normal-mode solutions is so important that it will be a theme throughout the course.



Exercises

*__3.1__ Starting with the Euler formula $e^{i\theta} = \cos(\theta) + i\sin(\theta)$ (and its complex conjugate), write $\cos(\theta)$ and $\sin(\theta)$ in terms of $e^{i\theta}$ and $e^{-i\theta}$.

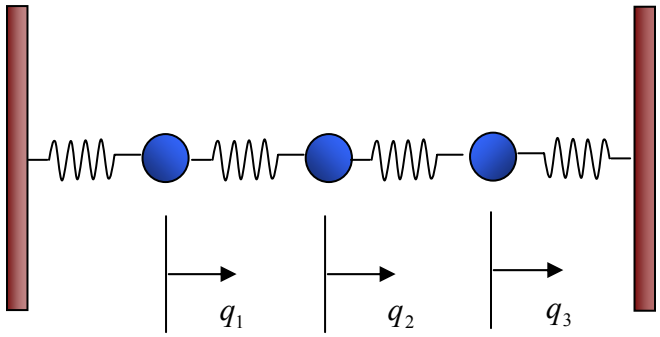
*__3.2__ Write the expression $Ae^{i\tilde{\omega}t} + Be^{-i\tilde{\omega}t}$ in the form $C\cos(\tilde{\omega}t) + D\sin(\tilde{\omega}t)$. That is, find C and D in terms of A and B. From this result show that if $B = A^*$ then C and D are both real (which means that $Ae^{i\tilde{\omega}t} + Be^{-i\tilde{\omega}t}$ is real).

*__3.3__ In the graph of the first normal-mode solution, $q_1(t)$ and $q_2(t)$ both look like cosine functions. Show for $A_1 = B_1 = 1/2$, that the solution

$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\left(A_1 e^{i\tilde{\omega}t} + B_1 e^{-i\tilde{\omega}t}\right)$ can indeed be written as $\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\cos(\tilde{\omega}t)$.

*__3.4__ If we take the limit $k_s' \to 0$ in the coupled oscillator problem, what does this correspond to physically? What happens to the normal mode frequencies? Does this make sense? (Note: if two normal modes have the same frequency, then they are said to be degenerate, and any linear combination of those two normal modes is also a normal mode.)

**__3.5 Three coupled oscillators__. In this problem you will find the normal modes of three coupled oscillators, as illustrated below. Assume that each object has mass m and each spring constant is k_s.



(The following steps lead you through the same procedure as is used in the notes to solve the two-oscillator problem in order to solve this problem. It will be most helpful if you carefully study that procedure before tackling this problem.)

(**a**) Using Newton's second law, write down the equation of motion for each object [in the form of Eq. (4) in the notes].
(**b**) Assume a normal-mode type solution and find the three algebraic equations [equivalent to Eq. (7) in the notes] that govern Ω^2 and the amplitudes q_{01}, q_{02}, and q_{03}.
(**c**) Write your equations in (**b**) in matrix form [equivalent to Eq. (9) in the notes].
(**d**) Find the characteristic equation [equivalent to Eq. (11) in the notes] that determines the three eigenvalues. (Hint: you will need to calculate the determinant of a 3×3 matrix.)
(**e**) Solve the characteristic equation and show that the three eigenvalues for this problem are $\Omega^2 = \left(2-\sqrt{2}\right)\tilde{\omega}^2, 2\,\tilde{\omega}^2, \left(2+\sqrt{2}\right)\tilde{\omega}^2$.
(**f**) For each eigenvalue, find the eigenvector associated with that eigenvalue.
(**g**) Write down the 3 normal mode solutions in the form of Eqs. (21) and (28) in the notes.
(**h**) As precisely as possible, describe the motion of the three objects for each of the normal modes.

Normal Mode Coordinates / Initial Value Problem

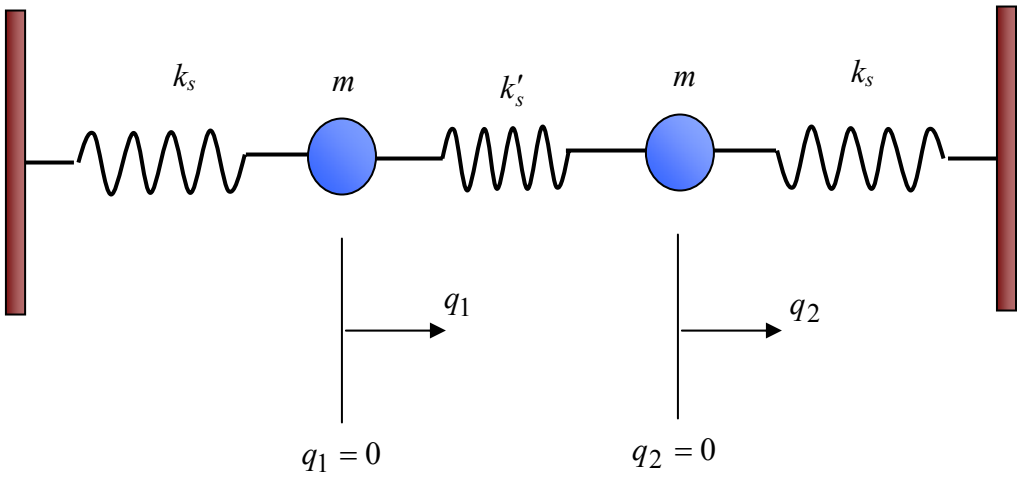
Overview and Motivation: We continue to look at the coupled-oscillator problem. We extend our analysis of this problem by introducing functions known as normal-mode coordinates. These coordinates make the coupled-oscillator problem simple because they transform the coupled equations of motion into two uncoupled equations of motion. Using the normal modes, we then solve the general initial-value problem for this system.

Key Mathematics: We gain experience with linear transformations and initial value problems.

I. Normal Mode Solutions

A. Summary from Last Lecture

The problem that we studied last time is shown in the following diagram. There are two objects, each with mass m and three springs. The springs on the ends have spring constant k_s and the one in the center has spring constant k_s'.



Last time we found the two normal-mode solutions, which can be written as

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \left(A_1 e^{i\Omega_1 t} + B_1 e^{-i\Omega_1 t} \right) \tag{1}$$

and

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}\left(A_2 e^{i\Omega_2 t} + B_2 e^{-i\Omega_2 t}\right), \tag{2}$$

where $\Omega_1 = \tilde{\omega}$ and $\Omega_2 = \sqrt{\tilde{\omega}^2 + 2\tilde{\omega}'^2}$ are the normal-mode frequencies of oscillation. As we will show below, any solution to this problem can be written as a linear combination of these two normal modes. Thus, we can write the most general solution to this problem as

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\left(A_1 e^{i\Omega_1 t} + B_1 e^{-i\Omega_1 t}\right) + \begin{pmatrix} 1 \\ -1 \end{pmatrix}\left(A_2 e^{i\Omega_2 t} + B_2 e^{-i\Omega_2 t}\right) \tag{3}$$

B. Normal Mode Coordinates

Let's now consider the following **linear transformation**[1] of the displacements $q_1(t)$ and $q_2(t)$,

$$\begin{pmatrix} Q_1(t) \\ Q_2(t) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix}\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix}. \tag{4}$$

Calculating the rhs of Eq. (4) produces[2]

$$\begin{pmatrix} Q_1(t) \\ Q_2(t) \end{pmatrix} = \frac{1}{2}\begin{pmatrix} q_1(t) + q_2(t) \\ q_1(t) - q_2(t) \end{pmatrix}. \tag{5}$$

Written more pedantically, we have

$$Q_1(t) = \frac{q_1(t) + q_2(t)}{2} \tag{6a}$$

and

$$Q_2(t) = \frac{q_1(t) - q_2(t)}{2}. \tag{6b}$$

For reasons that will soon become apparent, the functions $Q_1(t)$ and $Q_2(t)$ are known

[1] Any linear transformation of an N-vector can be represented as lhs multiplication of that vector by an $N \times N$ matrix.

[2] Note that the normal-mode coordinate Q_2 as defined here is the negative of Q_2 as defined in Dr. Torre's text *FWP*. We define it here with this change so as to be more consistent with the later treatment of N coupled oscillators. To be honest, it also makes some of the equations look prettier!

as **normal-mode coordinates**. (Why aren't they called normal-mode functions? Don't ask me!)

Let's now apply the linear transformation in Eq. (4) to the rhs of Eq. (3) and see what it tells us. Applying the transformation and equating the result to the lhs of Eq. (4) yields

$$\begin{pmatrix} Q_1(t) \\ Q_2(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\left(A_1 e^{i\Omega_1 t} + B_1 e^{-i\Omega_1 t}\right) + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\left(A_2 e^{i\Omega_2 t} + B_2 e^{-i\Omega_2 t}\right). \tag{7}$$

This equation may look complicated, but, in fact, it is very simple. It says that $Q_1(t)$ harmonically oscillates at the first normal-mode frequency Ω_1 and that $Q_2(t)$ harmonically oscillates at the second normal-mode frequency Ω_2. Pretty cool! In fact, if Eq. (3) is the general solution to this problem (more on this below), Eq. (7) say that no matter what the motion, the sum $q_1(t)+q_2(t)$ always oscillates at Ω_1, and the difference $q_1(t)-q_2(t)$ always oscillates at Ω_2.

C. Equations of Motion

Let's now go back to the coupled equations of motion,

$$\ddot{q}_1 + \tilde{\omega}^2 q_1 + \tilde{\omega}'^2(q_1 - q_2) = 0 \tag{8a}$$

and

$$\ddot{q}_2 + \tilde{\omega}^2 q_2 + \tilde{\omega}'^2(q_2 - q_1) = 0, \tag{8b}$$

and see what happens if we write them in terms of the normal-mode coordinates $Q_1(t)$ and $Q_2(t)$. To do that we need the **inverse** of the transformation in Eq. (4). Using

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix}^{-1} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{9}$$

(make sure that you understand this!) we apply this inverse transformation to Eq. (4), which gives us (after switching the rhs and lhs)

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = \begin{pmatrix} Q_1(t)+Q_2(t) \\ Q_1(t)-Q_2(t) \end{pmatrix}. \tag{10}$$

That is, $q_1(t) = Q_1(t) + Q_2(t)$ and $q_2(t) = Q_1(t) - Q_2(t)$. Substituting these results into Eq. (8) produces

$$\ddot{Q}_1 + \ddot{Q}_2 + \tilde{\omega}^2(Q_1 + Q_2) + 2\tilde{\omega}'^2 Q_2 = 0 \tag{11a}$$

and

$$\ddot{Q}_1 - \ddot{Q}_2 + \tilde{\omega}^2(Q_1 - Q_2) - 2\tilde{\omega}'^2 Q_2 = 0\,. \tag{11b}$$

Looks pretty ugly, eh? Well , it is about to get much simpler. If we take the sum and difference of Eqs. (11a) and (11b) we get the following two equations,

$$\ddot{Q}_1 + \tilde{\omega}^2 Q_1 = 0 \tag{12a}$$

and

$$\ddot{Q}_2 + (\tilde{\omega}^2 + 2\tilde{\omega}'^2)Q_2 = 0\,. \tag{12b}$$

First, notice that these two equations are uncoupled: the equation of motion for Q_1 doesn't depend upon Q_2 and vice-versa. Furthermore, you should now able to recognize each of these equations as the equation of motion for a single harmonic oscillator! Thus, Eq. (12a) tells us that Q_1 harmonically oscillates at $\tilde{\omega}$ $(=\Omega_1)$, and Eq. (12b) tells us that Q_2 harmonically oscillates at $\sqrt{\tilde{\omega}^2 + 2\tilde{\omega}'^2}$ $(=\Omega_2)$. Of course, this is exactly what was expressed earlier by Eq. (7).

We can also infer something very important from this transformation. Because the normal coordinates are governed by Eq. (12), which is simply an harmonic oscillator equation for each coordinate, we know that the general solution for $Q_1(t)$and $Q_2(t)$ is given by Eq. (7). Thus, the general solution for $q_1(t)$and $q_2(t)$ is given by the inverse transformation of Eq. (7), which is simply Eq. (3). This proves that the general solution for $q_1(t)$ and $q_2(t)$ is, indeed, a linear combination of the normal mode coordinates $Q_1(t)$and $Q_2(t)$. This is a general result that we will use throughout the course.

II. Initial Value Problem

Let's now solve the initial-value problem for the coupled-oscillator system. That is, we want to write Eq. (3), the general solution to the coupled oscillator problem, in terms of the initial conditions $q_1(0)$, $\dot{q}_1(0)$, $q_2(0)$, and $\dot{q}_2(0)$ (which are all real quantities).

Now Eq. (3),

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\left(A_1 e^{i\Omega_1 t} + B_1 e^{-i\Omega_1 t}\right) + \begin{pmatrix} 1 \\ -1 \end{pmatrix}\left(A_2 e^{i\Omega_2 t} + B_2 e^{-i\Omega_2 t}\right), \tag{3}$$

uses the complex form of the harmonic oscillator solution. Looking back on p. 8 of the Lecture 2 notes, we see that we have three choices about how to deal with making the IVP solution real. Let's use the first approach and make Eq. (3) manifestly real by setting $B_1 = A_1^*$ and $B_2 = A_2^*$. Then we have

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\left(A_1 e^{i\Omega_1 t} + A_1^* e^{-i\Omega_1 t}\right) + \begin{pmatrix} 1 \\ -1 \end{pmatrix}\left(A_2 e^{i\Omega_2 t} + A_2^* e^{-i\Omega_2 t}\right). \tag{13}$$

This expression is real because each term in parenthesis is the sum of a complex number and its complex conjugate. To rewrite Eq. (13) in a form that is explicitly real we use the relationship

$$Ae^{ix} + A^* e^{-ix} = 2\,\mathrm{Re}\left(Ae^{ix}\right) = 2\left[\mathrm{Re}(A)\cos(x) - \mathrm{Im}(A)\sin(x)\right], \tag{14}$$

so that Eq. (13) becomes

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = 2\begin{pmatrix} 1 \\ 1 \end{pmatrix}\left[\mathrm{Re}(A_1)\cos(\Omega_1 t) - \mathrm{Im}(A_1)\sin(\Omega_1 t)\right] + 2\begin{pmatrix} 1 \\ -1 \end{pmatrix}\left[\mathrm{Re}(A_2)\cos(\Omega_2 t) - \mathrm{Im}(A_2)\sin(\Omega_2 t)\right]. \tag{15}$$

We now apply the initial conditions to Eq. (15), which gives us

$$\begin{pmatrix} q_1(0) \\ q_2(0) \end{pmatrix} = 2\begin{pmatrix} 1 \\ 1 \end{pmatrix}\mathrm{Re}(A_1) + 2\begin{pmatrix} 1 \\ -1 \end{pmatrix}\mathrm{Re}(A_2), \tag{16}$$

and

$$\begin{pmatrix} \dot{q}_1(0) \\ \dot{q}_2(0) \end{pmatrix} = -2\Omega_1\begin{pmatrix} 1 \\ 1 \end{pmatrix}\mathrm{Im}(A_1) - 2\Omega_2\begin{pmatrix} 1 \\ -1 \end{pmatrix}\mathrm{Im}(A_2). \tag{17}$$

The easiest way to solve for the four unknowns [$\mathrm{Re}(A)$, $\mathrm{Im}(A)$, $\mathrm{Re}(C)$, and $\mathrm{Im}(C)$] is to apply the normal-mode transformation $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{pmatrix}$ to each side of these two equations, which produces

$$\frac{1}{2}\begin{pmatrix} q_1(0)+q_2(0) \\ q_1(0)-q_2(0) \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix}\mathrm{Re}(A_1)+2\begin{pmatrix} 0 \\ 1 \end{pmatrix}\mathrm{Re}(A_2), \tag{18}$$

and

$$\frac{1}{2}\begin{pmatrix} \dot{q}_1(0)+\dot{q}_2(0) \\ \dot{q}_1(0)-\dot{q}_2(0) \end{pmatrix} = -2\Omega_1\begin{pmatrix} 1 \\ 0 \end{pmatrix}\mathrm{Im}(A_1)-2\Omega_2\begin{pmatrix} 0 \\ 1 \end{pmatrix}\mathrm{Im}(A_2). \tag{19}$$

From these last two equations we immediately see that

$$\mathrm{Re}(A_1) = \frac{q_1(0)+q_2(0)}{4}, \tag{20a}$$

$$\mathrm{Im}(A_1) = -\frac{\dot{q}_1(0)+\dot{q}_2(0)}{4\Omega_1}, \tag{20b}$$

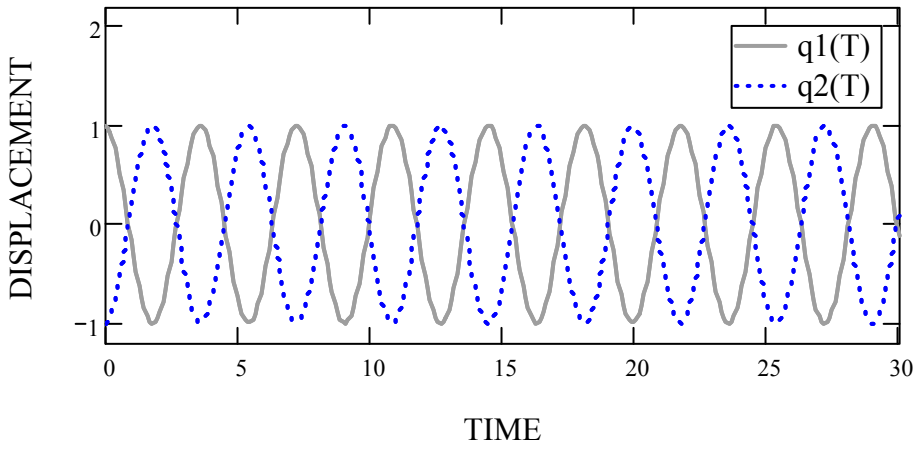
$$\mathrm{Re}(A_2) = \frac{q_1(0)-q_2(0)}{4}, \text{ and} \tag{20c}$$

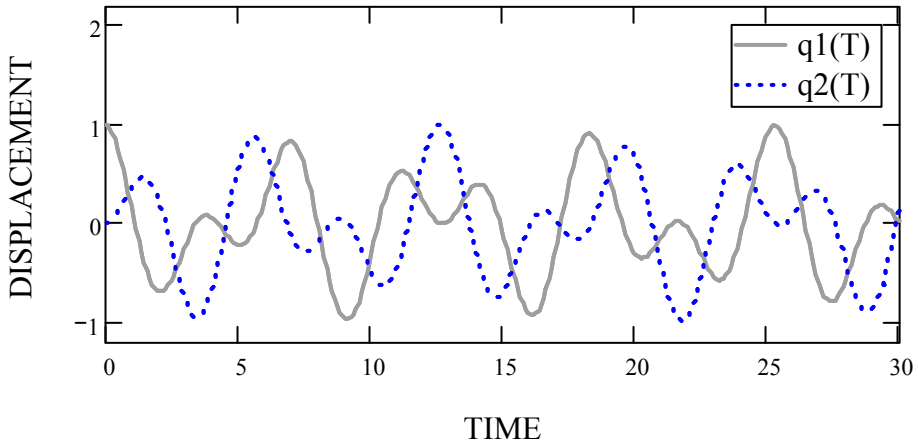
$$\mathrm{Im}(A_2) = \frac{\dot{q}_2(0)-\dot{q}_1(0)}{4\Omega_2}. \tag{20d}$$

If we now substitute Eq. (20) into Eq. (15) we finally obtain the solution to the IVP,

$$\begin{aligned}\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = {} & \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\left\{[q_1(0)+q_2(0)]\cos(\Omega_1 t)+\left[\frac{\dot{q}_1(0)+\dot{q}_2(0)}{\Omega_1}\right]\sin(\Omega_1 t)\right\} \\ & +\frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\left\{[q_1(0)-q_2(0)]\cos(\Omega_2 t)+\left[\frac{\dot{q}_1(0)-\dot{q}_2(0)}{\Omega_2}\right]\sin(\Omega_2 t)\right\}\end{aligned}. \tag{21}$$

The graphs on the following page illustrate the motion that results for two sets of initial conditions. For both graphs $m=1$, $k_s=1$, and $k_s'=1$ (so that $\Omega_1=1$ and $\Omega_2=\sqrt{3}$). In the top graph $q_1(0)=1$, $q_2(0)=-1$, $\dot{q}_1(0)=0$, and $\dot{q}_2(0)=0$. What special motion is this? In the second graph the initial conditions are $q_1(0)=1$, $q_2(0)=0$, $\dot{q}_1(0)=0$, and $\dot{q}_2(0)=0$. This motion is quite complicated. In fact, it is not even periodic: it never repeats, even though the normal-mode coordinates are simply harmonically oscillating at their respective frequencies. The nonrepetitive nature of the motion occurs because (in this example) the ratio is of the two normal-mode frequencies is not a rational number.





Exercises

*__4.1__ Apply the inverse transformation $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ to Eq. (7) to recover Eq. (3).

*__4.2__ Assuming $q_1(0)=0$ and $q_2(0)=0$, find the general condition on the initial velocities $\dot{q}_1(0)$ and $\dot{q}_2(0)$ that results in only the first normal mode being excited.

*__4.3__ Assuming $q_1(0)=0$ and $q_2(0)=0$, find the general condition on the initial velocities $\dot{q}_1(0)$ and $\dot{q}_2(0)$ that results in only the second normal mode being excited.

**__4.4__ The general solution to the two-coupled oscillator problem can alternatively be expressed in terms of real quantities as

$$\begin{pmatrix} q_1(t) \\ q_2(t) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \left[A\cos(\Omega_1 t) + B\sin(\Omega_1 t) \right] + \begin{pmatrix} 1 \\ -1 \end{pmatrix} \left[C\cos(\Omega_2 t) + D\sin(\Omega_2 t) \right]$$

Starting with this form of the general solution find the (real) parameters A, B, C, and D in terms of the initial conditions $q_1(0)$, $\dot{q}_1(0)$, $q_2(0)$, and $\dot{q}_2(0)$. Check to see that your solution agrees with Eq. (21).

*__4.5__ Use Euler's relation to derive Eq. (14).

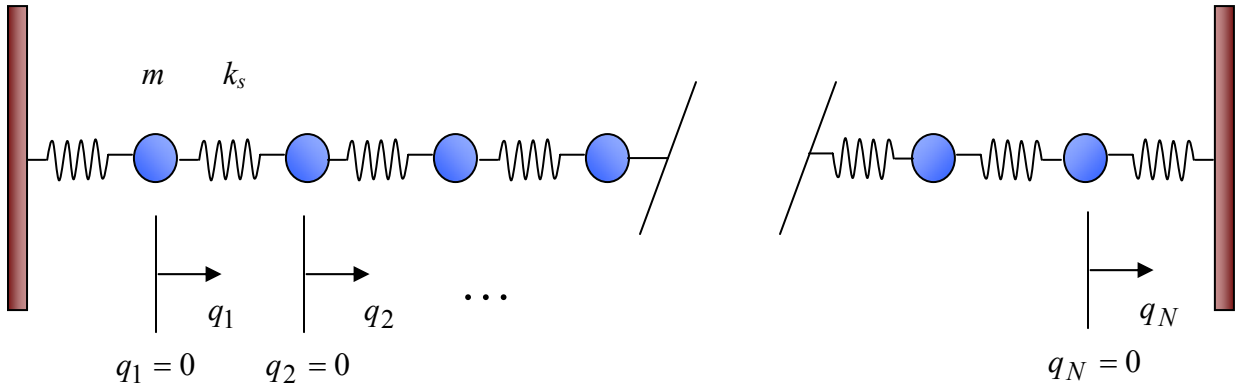
Linear Chain / Normal Modes

Overview and Motivation: We extend our discussion of coupled oscillators to a chain of N oscillators, where N is some arbitrary number. When N is large it will become clear that the normal modes for this system are essentially standing waves.

Key Mathematics: We gain some more experience with matrices and eigenvalue problems.

I. The Linear Chain of Coupled Oscillators

Because two oscillators are never enough, we now extend the system that we have discussed in the last two lectures to N coupled oscillators, as illustrated below. For this problem we assume that all objects have the same mass m and all springs have the same spring constant k_s.



Our first goal is to find the normal modes of this system. At the beginning we approach this problem in the same manner as for two coupled oscillators: we find the net force on each oscillator, find each equation of motion, and then assume a normal-mode type solution for the system. Let's consider some arbitrary object in this chain, say the jth object. The force on this object will depend upon the stretch of the two springs on either side of it. With a little thought, you should be able to write down the net force on this object as

$$F_j = -k_s\left(q_j - q_{j-1}\right) - k_s\left(q_j - q_{j+1}\right), \tag{1}$$

or, upon simplifying,

$$F_j = k_s\left(q_{j-1} - 2q_j + q_{j+1}\right). \tag{2}$$

You might worry that this equation is not valid for the first ($j=1$) and last ($j=N$) objects, but if we assume that the $j=0$ and $j=N+1$ objects (the walls) have infinite mass so that q_0 and q_{N+1} are identically zero, then Eq. (2) applies to all N objects. We shall refer to these two conditions, $q_0=0$ and $q_{N+1}=0$, as **boundary conditions** (bc's) on the chain of oscillators.

With the expression for the net force on each object we can write down the equation of motion (Newton's second law!) for each object as

$$\ddot{q}_j - \tilde{\omega}^2\left(q_{j-1} - 2q_j + q_{j+1}\right) = 0\,, \tag{3}$$

where $1 \le j \le N$ and, as before, $\tilde{\omega}^2 = k_s/m$. Notice that each equation of motion is coupled: the equation of motion for the j th object depends upon the displacement of both the $(j-1)$ and $(j+1)$ objects.

II. Normal Mode Solutions

We now look for normal-mode solutions (where all masses oscillate at the same frequency) by assuming that[1]

$$q_j = q_{0,j}e^{i\Omega t}\,. \tag{4}$$

If we substitute Eq. (4) into Eq. (3), after a bit of algebra the equations of motion become

$$\Omega^2 q_{0,j} + \tilde{\omega}^2\left(q_{0,j-1} - 2q_{0,j} + q_{0,j+1}\right) = 0 \tag{5}$$

Now, keep in mind that what we have here are N equations of motion, one for each value of j from 1 to N. As in the two-oscillator problem, the set of equations can be expressed in matrix notation

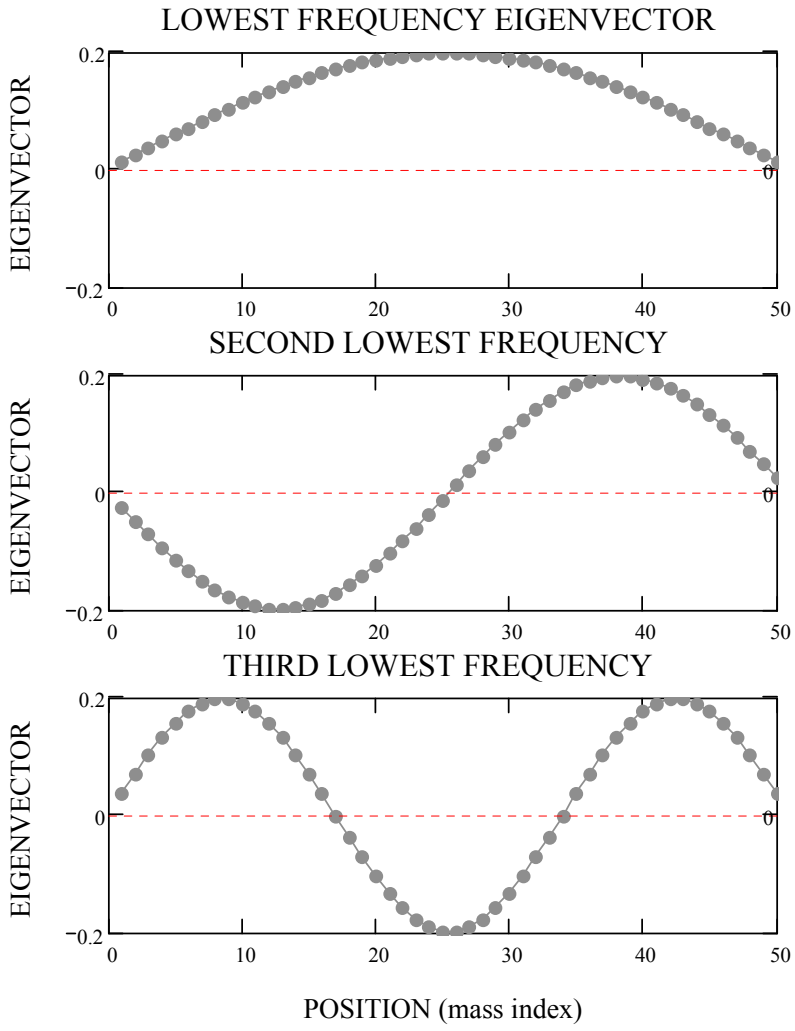
$$\begin{pmatrix} 2\tilde{\omega}^2 & -\tilde{\omega}^2 & 0 & 0 & \\ -\tilde{\omega}^2 & 2\tilde{\omega}^2 & -\tilde{\omega}^2 & 0 & \\ 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2 & -\tilde{\omega}^2 & \cdots \\ 0 & 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2 & \\ & & \vdots & & \end{pmatrix}\begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ q_{0,4} \\ \vdots \end{pmatrix} = \Omega^2\begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ q_{0,4} \\ \vdots \end{pmatrix} \tag{6}$$

[1] We have slightly changed notation here. We now write the amplitudes $q_{0,j}$ with a comma between the zero and the mass index so that terms such as $q_{0,j+1}$ are unambiguous.

or

$$\begin{pmatrix} 2\tilde{\omega}^2-\Omega^2 & -\tilde{\omega}^2 & 0 & 0 & \\ -\tilde{\omega}^2 & 2\tilde{\omega}^2-\Omega^2 & -\tilde{\omega}^2 & 0 & \\ 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2-\Omega^2 & -\tilde{\omega}^2 & \cdots \\ 0 & 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2-\Omega^2 & \\ & & \vdots & & \end{pmatrix} \begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ q_{0,4} \\ \vdots \end{pmatrix} = 0 \qquad (7)$$

So, as before, finding the normal modes reduces to finding eigenvalues Ω^2 and eigenvectors $\begin{pmatrix} q_{0,1} \\ q_{0,2} \\ \vdots \end{pmatrix}$ [of the $N \times N$ matrix in Eq. (6)]. Recall that the eigenvalues are found by solving the (characteristic) equation that arises when we set the determinant of the $N \times N$ matrix in Eq. (7) to zero.



A. Eigenvectors

Now for N any larger than 3 solving the characteristic equation for the eigenvalues and eigenvectors by hand is not advisable. So let's turn to a computer mathematics program, such as Mathcad, and see what insight we can gain into this problem. Given the matrix in Eq. (6) (with a specific value for $\tilde{\omega}^2$), Mathcad can calculate the eigenvalues and eigenvectors of that matrix. In the graphs on the previous page we plot the eigenvectors corresponding to the three lowest eigenvalues for the $N = 50$ problem.

The key thing to notice is that these eigenvectors look like standing waves (on a string, for example). That is, as a function of position (i.e., mass index) j, the components $q_{0,j}$ of the eigenvector appear to be a sine function [which must equal zero at the ends of the chain ($j = 0$ and $j = N+1$) because of the bc's].

This observation inspires the following ansatz for the eigenvectors

$$q_{0,j} = A\sin(\phi\, j), \tag{8}$$

where A is some arbitrary **amplitude** for this sine function (it could be complex because we are dealing with a complex form of the solutions), and ϕ is some real number that will be different for each normal mode.[2] Now Eq. (8) obviously satisfies the $q_0 = 0$ bc on the lhs of chain, but not necessarily the rhs bc $q_{N+1} = 0$. To satisfy this bc we must have

$$q_{0,N+1} = A\sin[\phi(N+1)] = 0, \tag{9}$$

which is true only for $\phi(N+1) = n\pi$, where n is an integer. That is, we must have

$$\phi_n = \frac{n\pi}{N+1} \tag{10}$$

where the integer n labels the (normal-mode) solution. Now because any integer n in Eq. (10) produces a value for ϕ that satisfies Eq. (9), it looks like ϕ_n can take on an infinite number of values; this seems to imply an infinite number of normal modes. Well, this can't be right because we know that there are only two normal modes for

[2] Recall, for a standing wave on a string the spatial part of the standing wave can be written as $\sin\left(\frac{2\pi}{\lambda}x\right)$, so the parameter ϕ is obviously related to the wavelength of the normal modes (in some manner – more detail on this later).

the two-oscillator problem. In fact, because the N oscillator problem involves an N dimensional eigenvalue problem, there are exactly N normal modes. The solution to this conundrum lies in the fact that the sine function [in Eq. (9)] is periodic. It can be shown that there are $N+1$ unique solutions, but because the $n=0$ solution is trivial, there are only N unique, nontrivial solutions. In fact, we can specify these N unique solutions by choosing n such that

$$1 \le n \le N . \tag{11}$$

Combining Eqs. (8), (10), and (11) we can write the N eigenvectors as

$$q_{0,j} = A\sin\left(\frac{n\pi}{N+1}j\right), \qquad 1 \le n \le N \tag{12}$$

B. Eigenvalues

So we have now specified the eigenvectors. What about the eigenvalues? We can obtain these by inserting Eq. (8) into Eq. (5), which produces

$$\Omega^2 \sin(\phi j) + \tilde{\omega}^2 \{\sin[\phi(j-1)] - 2\sin(\phi j) + \sin[\phi(j+1)]\} = 0 . \tag{13}$$

Now it looks like this equation depends upon j, but it does not. Using some trig identities it is not difficult to show that Eq. (13) simplifies and can be solved for Ω^2 as

$$\Omega^2 = 4\tilde{\omega}^2 \sin^2\left(\frac{\phi}{2}\right). \tag{14}$$

And remembering that ϕ only takes on the discrete values given by Eq. (10), we have the N eigenvalues

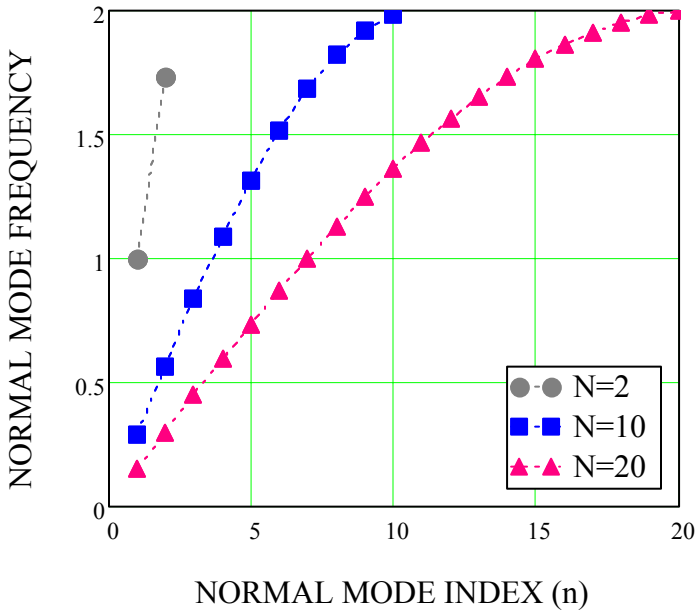
$$\Omega_n^2 = 4\tilde{\omega}^2 \sin^2\left(\frac{n\pi}{2(N+1)}\right), \tag{15}$$

where $n = 1, 2, 3, \cdots, N$. The normal-mode frequencies are thus given by

$$\Omega_{n\pm} = \pm 2\tilde{\omega}\sin\left(\frac{n\pi}{2(N+1)}\right). \tag{16}$$

It is interesting to plot the (positive) frequencies as a function of mode number n. Such a graph is shown below for several values of N. As with previous graphs we have set $m=1$ and $k_s = 1$.

As we will discuss in the next lecture, these graphs are essentially graphs of frequency vs inverse wavelength, and as such are known as **dispersion relations** or **dispersion curves**. As we will see as we work our way through the course, the dispersion relation is extremely useful in understanding the propagation of waves associated with that dispersion relation. Also, as we will discuss in the next lecture, the dispersion relation also contains information on the interactions between (the springs connecting)



the oscillating objects. Notice that the frequencies plotted for two oscillators ($N=2$) equal our previous results $\Omega_1 = 1$ and $\Omega_2 = \sqrt{3}$ (for the special case of $m=1$ and $k_s = 1$).

III. The Initial Value Problem

Lastly, we discuss how the initial value problem can be solved using the normal modes. Quite generally, using the above results and including both the Ω_{n+} and Ω_{n-} frequencies, we can write the n th normal-mode solution as

$$\begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix}_n = \begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix} \left(A_n e^{i\Omega_n t} + B_n e^{-i\Omega_n t}\right) \qquad (17)$$

where $\Omega_n = \Omega_{n+}$, and the constants A_n and B_n (which have replaced A above) are arbitrary complex numbers.[3] The general solution can thus be written as a linear combination of the normal modes as

$$\begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix} = \sum_{n=1}^{N} \left[\begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix} \left(A_n e^{i\Omega_{n+}t} + B_n e^{-i\Omega_{n+}t} \right) \right]. \tag{18}$$

[Equation (18) is the extension of Eq. (3) of the Lecture (4) notes.] As before, the arbitrary amplitudes A_n and B_n depend upon the initial conditions of all the oscillating objects.

To see exactly how the A_n and B_n are determined, let's consider the $N = 3$ case. As in the two-oscillator case, let's make the normal modes explicitly real by setting $B_n = A_n^*$. For three oscillators Eq. (18) then becomes

$$\begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \end{pmatrix} = \sum_{n=1}^{3} \begin{pmatrix} \sin\left(\frac{n\pi}{4}1\right) \\ \sin\left(\frac{n\pi}{4}2\right) \\ \sin\left(\frac{n\pi}{4}3\right) \end{pmatrix} \left(A_n e^{i\Omega_n t} + A_n^* e^{-i\Omega_n t} \right) \tag{19}$$

As in Lecture Notes 4 for the two-oscillator problem, we can rewrite $A_n e^{i\Omega_n t} + A_n^* e^{-i\Omega_n t}$ as $2[\mathrm{Re}(A_n)\cos(\Omega_n t) - \mathrm{Im}(A_n)\sin(\Omega_n t)]$ and apply the initial conditions, which gives us

$$\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \end{pmatrix} = \sum_{n=1}^{3} 2 \begin{pmatrix} \sin\left(\frac{n\pi}{4}1\right) \\ \sin\left(\frac{n\pi}{4}2\right) \\ \sin\left(\frac{n\pi}{4}3\right) \end{pmatrix} \mathrm{Re}(A_n), \tag{20}$$

and

$$\begin{pmatrix} \dot{q}_1(0) \\ \dot{q}_2(0) \\ \dot{q}_3(0) \end{pmatrix} = \sum_{n=1}^{3} -2\Omega_n \begin{pmatrix} \sin\left(\frac{n\pi}{4}1\right) \\ \sin\left(\frac{n\pi}{4}2\right) \\ \sin\left(\frac{n\pi}{4}3\right) \end{pmatrix} \mathrm{Im}(A_n). \tag{21}$$

[3] Notice that the column vector of the rhs of Eq. (17) is the n th eigenvector of the associated eigenvalue problem.

So we see that the real part of the amplitudes A_n depend upon the initial positions of the three objects, while the imaginary part of the amplitudes depend upon their initial velocities. So where do we go from here? You may remember that for the two-oscillator problem we applied the normal-mode transformation to the equivalent of Eqs. (20) and (21), which allowed us to find the amplitudes (see p. 5-6 of the Lecture 4 notes). There is an equivalent transformation here that will allow us to find the A_n's. To most easily see what it is, let's explicitly write out Eq. (20) as

$$\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \end{pmatrix} = 2\left[\begin{pmatrix} \sin\left(\frac{\pi}{4}\right) \\ \sin\left(\frac{\pi}{2}\right) \\ \sin\left(\frac{3\pi}{4}\right) \end{pmatrix} \mathrm{Re}(A_1) + \begin{pmatrix} \sin\left(\frac{\pi}{2}\right) \\ \sin(\pi) \\ \sin\left(\frac{3\pi}{2}\right) \end{pmatrix} \mathrm{Re}(A_2) + \begin{pmatrix} \sin\left(\frac{3\pi}{4}\right) \\ \sin\left(\frac{3\pi}{2}\right) \\ \sin\left(\frac{9\pi}{4}\right) \end{pmatrix} \mathrm{Re}(A_3) \right], \tag{22}$$

and evaluate the sine functions, which gives us

$$\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \end{pmatrix} = \left[\begin{pmatrix} \sqrt{2} \\ 2 \\ \sqrt{2} \end{pmatrix} \mathrm{Re}(A_1) + \begin{pmatrix} 2 \\ 0 \\ -2 \end{pmatrix} \mathrm{Re}(A_2) + \begin{pmatrix} \sqrt{2} \\ -2 \\ \sqrt{2} \end{pmatrix} \mathrm{Re}(A_3) \right]. \tag{23}$$

Now notice what now happens if we multiply this equation by the first eigenvector $\begin{pmatrix} \sin\left(\frac{\pi}{4}\right) \\ \sin\left(\frac{\pi}{2}\right) \\ \sin\left(\frac{3\pi}{4}\right) \end{pmatrix}$ when it is written as a row vector $\left(\sin\left(\frac{\pi}{4}\right) \quad \sin\left(\frac{\pi}{2}\right) \quad \sin\left(\frac{3\pi}{4}\right)\right) = \frac{1}{2}\left(\sqrt{2} \quad 2 \quad \sqrt{2}\right)$. We obtain

$$\frac{1}{2}\left(\sqrt{2}\, q_1(0) + 2q_2(0) + \sqrt{2}\, q_3(0)\right) = 4\,\mathrm{Re}(A_1). \tag{24}$$

Notice the very nice result that the terms containing the amplitudes A_2 and A_3 produce zero when multiplied by the first eigenvector (in row form). We can now solve for the real part of A_1 in terms of the initial positions as

$$\mathrm{Re}(A_1) = \frac{1}{8}\left(\sqrt{2}\, q_1(0) + 2q_2(0) + \sqrt{2}\, q_3(0)\right). \tag{25}$$

This equation is equivalent to the first row of Eq. (18) [or Eq. (20a)] in the Lecture 4 notes for the two-oscillator problem. To obtain $\mathrm{Re}(A_2)$ and $\mathrm{Re}(A_3)$ it should be obvious that one needs to multiply Eq. (23) by the respective (row) eigenvectors.

Further, to find the imaginary parts of the amplitudes, one similarly multiplies Eq. (21) by the row eigenvectors.

This "trick" of multiplying by the row eigenvector to obtain the corresponding amplitude is probably the most important part of this lecture. We will repeat it many times throughout the course: when we discuss Fourier series we will use this trick to find the Fourier coefficients of a function; when we talk about vector spaces this trick will be recognized as the "inner product"; and when we talk about Fourier transforms this trick will be known as "inversion". As we discuss these topics, you should keep in mind this little trick that allowed us to find the amplitudes A_n.

So we know how to find the A_n's, but what about the normal-mode transformation mentioned above? Well, it is lurking about here. If we now create an $N \times N$ matrix by stacking the row eigenvectors, then we indeed have that transformation. So for the three-oscillator problem, the transformation matrix would be

$$\frac{1}{2}\begin{pmatrix} \sqrt{2} & 2 & \sqrt{2} \\ 2 & 0 & -2 \\ \sqrt{2} & -2 & \sqrt{2} \end{pmatrix}. \tag{26}$$

If one multiples Eqs. (20) and (21) by Eq. (26) then one obtains two equations that are equivalent to Eqs. (18) and (19) of the Lecture 4 notes for the two-oscillator case. Also, if one multiplies the column vector $\begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \end{pmatrix}$ by Eq. (26) then one obtains the normal-mode coordinates $\begin{pmatrix} Q_1(t) \\ Q_2(t) \\ Q_3(t) \end{pmatrix}$ for the three-oscillator case.

Exercises

***5.1** Using the appropriate trig formulae, obtain Eq. (14) for Ω^2 from Eq. (13).

***5.2 Only N unique eigenvalues and eigenvectors**
Eqs. (12) and (15) specify the N eigenvector and eigenvalues for the N oscillator problem. The condition $1 \le n \le N$ implies that values of n outside of this range simply give a solution that is the same as one of the solutions inside the range $1 \le n \le N$.

(**a**) Starting with Eq. (15) and using the angle-addition formula for the sine function, show, for example, that Ω_{N+2}^2 is the same as Ω_N^2. [Hint: write N as $(N+1)-1$ and $N+2$ as $(N+1)+1$.]
(**b**) Starting with Eq. (12) show also that the eigenvector for $n = N+2$ is the same as the eigenvector for $n = N$.

*__5.3__ Similar to the second figure in the notes, graph the three eigenvectors for three coupled oscillators.

*__5.4 Four coupled oscillators__
(a) What are the eigenvalues Ω_n^2 for four coupled oscillators?
(b) Similar to the second figure in the notes, find and then graph the four eigenvectors for four coupled oscillators.

*__5.5__ Similar to Eq. (25), find the imaginary part of A_2 for the $N = 3$ system of coupled oscillators.

*__5.6__ Apply Eq. (26), the normal-mode transformation, to Eqs. (20) and (21) to obtain the two equations for three oscillators that are equivalent to Eqs. (18) and (19) of the Lecture 4 notes for two oscillators.

*__5.7__ Show that the square of Eq. (26), the normal-mode transformation, is proportional to the identity matrix. Thus find the inverse of the normal-mode transformation.

*__5.8__ For the three-oscillator problem find the normal-mode coordinates $Q_1(t)$, $Q_2(t)$, and $Q_3(t)$ in terms of the displacements $q_1(t)$, $q_2(t)$, and $q_3(t)$.

Traveling Waves, Standing Waves, and the Dispersion Relation

Overview and Motivation: We review the relationship between traveling and standing waves. We then discuss a general relationship that is important in all of wave physics – the relationship between oscillation frequency and wave vector – which is known as the dispersion relation.

Key Mathematics: We get some more practice with trig identities and eigenvalue problems.

I. Traveling and Standing Waves

A. Basic Definitions

The simplest definition of a 1D **traveling wave** is a function of the form

$$q_1(x,t) = g(x - ct) \tag{1a}$$

or

$$q_2(x,t) = f(x + ct), \tag{1b}$$

where c is some positive constant.[1] The constant c is the **speed of propagation** of the wave. The wave in Eq. (1a) propagates in the positive x direction, while the wave in Eq. (1b) propagates in the negative x direction. Now the functions g and f in Eq. (1) can essentially be any (well behaved) function, but often we are interested in **harmonic waves**. In this case the functions g and f in Eq. (1) take on the form

$$g(x - ct) = A\sin\left[\frac{2\pi}{\lambda}(x - ct) + \phi\right] \tag{2a}$$

and

$$f(x + ct) = B\sin\left[\frac{2\pi}{\lambda}(x + ct) + \psi\right], \tag{2b}$$

where A and B are the amplitudes, ϕ and ψ are the **phases**, and λ is the **wavelength** of the wave. Now the x- and t-dependent parts of the sine-function arguments are often written as $kx \pm \omega t$, and so we can identify the **wave vector** k as

[1] As we shall see, the functions in Eq. (1) are the general solutions to the wave equation, which we will study in short order. However, we shall also see, when we study the Schrödinger equation, that not all waves have these functional forms.

$$k = \frac{2\pi}{\lambda} \tag{3}$$

and the **angular frequency** ω as[2]

$$\omega = \frac{2\pi c}{\lambda}. \tag{4}$$

You should recall from freshman physics that the speed c, frequency $\nu = \omega/(2\pi)$ and wavelength λ are related by $\nu = c/\lambda$.

So what is a **standing wave**? Simply put, it is the superposition (i.e., sum) of two equal-amplitude, equal-wavelength (and thus equal-frequency) harmonic waves that are propagating in opposite directions. Using Eqs. (2), (3), and (4) (and for simplicity setting $\phi = \psi = 0$) we can write such a wave as

$$q_S(x,t) = A[\sin(kx - \omega t) + \sin(kx + \omega t)]. \tag{5}$$

With a bit of trigonometry, specifically the angle-addition formula for the sine function, Eq. (5) can be rewritten as

$$q_S(x,t) = 2A\sin(kx)\cos(\omega t) \tag{6}$$

So instead of being a function of $kx \pm \omega t$, a standing wave is a *product* of a function of x and a function of t. Equation (6) also show us how to identify the wave vector k and angular frequency ω in the case of an harmonic standing wave: whatever multiplies x is the wave vector and whatever multiplies t is the angular frequency.

In fact, for nonharmonic standing waves it is probably safe to define a standing wave as a wave where all parts of the system oscillate in phase, as is the case of the harmonic standing wave defined by Eq. (6).

B. Connection to the Coupled Oscillator Problem

Let's now go back to the coupled oscillator problem, and reconsider the nth normal-mode solutions to that problem, which we previously wrote as

[2] Do not confuse this definition of ω (the angular frequency of the wave) with our earlier definition of $\tilde{\omega}$ ($=\sqrt{k/m}$) that arises when discussing single or coupled harmonic oscillators. It is easy to confuse the two definitions because for a single harmonic oscillator $\tilde{\omega}$ is also an angular frequency.

$$\begin{pmatrix} q_1(t) \\ q_2(t) \\ q_3(t) \\ \vdots \\ q_N(t) \end{pmatrix}_n = \begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix} \left(A_n e^{i\Omega_n t} + B_n e^{-i\Omega_n t}\right), \tag{7}$$

where $\Omega_n = 2\tilde{\omega}\sin\left[n\pi/2(N+1)\right]$. As we mentioned last time, these modes are essentially standing waves. Let's see that this is the case by writing Eq. (7) in the form of Eq. (6). After we do this, let's also identify the wave vector k and frequency ω for the normal modes. As written, Eq. (7) explicitly lists the motion of each individual oscillator. But the nth normal mode can also be written as a function of object index j and time t as

$$q_{(n)}(j,t) = \sin\left(\frac{n\pi}{N+1}j\right)\left(A_n e^{i\Omega_n t} + B_n e^{-i\Omega_n t}\right), \tag{8}$$

where j labels the oscillator. Although j is a discrete index, we have included it in the argument of the normal-mode function because it is the variable that labels position along the chain. Equation (8) is almost in the form of Eq. (6). In fact, if we take the specialized case of $A_n = B_n = A$, where A is real, then Eq. (8) can be written as

$$q_{(n)}(j,t) = 2A\sin\left(\frac{n\pi}{N+1}j\right)\cos(\Omega_n t). \tag{9}$$

This is very close, except in Eq. (6) the position variable is the standard distance variable x, while in Eq. (9) we are still using the object index j to denote position. However, if we define the equilibrium distance between nearest-neighbor objects as d, then we can connect x and j via $x = jd$, and so we can rewrite Eq. (9) as

$$q_{(n)}(x,t) = 2A\sin\left(\frac{n\pi}{N+1}\frac{x}{d}\right)\cos(\Omega_n t). \tag{10}$$

Now, remembering that whatever multiplies x is the wave vector k and that whatever multiplies t is the angular frequency ω, we have

$$k = \frac{n\pi}{N+1}\frac{1}{d} \tag{11}$$

and

$$\omega = \Omega_n = 2\tilde{\omega}\sin\left(\frac{n\pi}{2(N+1)}\right) \tag{12}$$

for the coupled-oscillator standing waves.

III. Dispersion Relations

A. Definition and Some Simple Examples

Simply stated, a **dispersion relation** is the function $\omega(k)$ for an harmonic wave. For the simplest of waves, where the speed of propagation c is a constant, we see from Eqs. (3) and (4) that their dispersion relation is simply

$$\omega(k) = ck\,. \tag{13}$$

That is, the frequency ω is a linear function of the wave vector k. We also see from Eq.(13) that the ratio ω/k is simply the propagation speed c. As we will discuss in more detail in a later lecture, the ratio ω/k is technically known as the **phase velocity**.[3]

Now you may be thinking, what is the big deal here? – Eq. (13) is so simple, what could be interesting about it? Now it is simple if the phase velocity c is independent of k. But this is usually not the case. Recall, for example, the propagation of light in a dielectric medium (such as glass) where the index of refraction $n = c_0/c$ (where c_0 is the speed of light in a vacuum) depends upon the wavelength (and thus the wave vector).[4] In this case Eq. (13) becomes

$$\omega(k) = \frac{c_0}{n(k)}k\,. \tag{14}$$

The dispersion relation now has the possibility of being quite interesting.

Another example of an interesting, nonlinear dispersion relation is found in modern physics. In your modern-physics class you (hopefully!) studied solutions to the Schrödinger equation. The wave (function) that describes a free particle (one with no

[3] OK, it should probably be called the phase speed, but it isn't. Sorry, even in physics all quantities are not logically named.

[4] The dependence of the phase velocity on wave vector leads to dispersion of light by a prism, for example. Thus the name "dispersion relation".

net force acting on it) propagating in the x direction with momentum p can be written as

$$\psi_p(x,t) = \psi_0 e^{i\left(\frac{p}{\hbar}x - \frac{p^2}{2m\hbar}t\right)}, \tag{15}$$

where m is the mass of the particle and $\hbar$ is Planck's constant. Comparing Eq. (15) with Eq. (5), for example, we identify the wave vector

$$k = \frac{p}{\hbar} \tag{17}$$

and the frequency

$$\omega = \frac{p^2}{2m\hbar}. \tag{18}$$

The dispersion relation is thus

$$\omega(k) = \frac{\hbar k^2}{2m}. \tag{19}$$

Notice that this dispersion relation is quadratic in the wave vector k. As we will study later, a nonlinear dispersion relation has profound consequences for the propagation of a localized wave (often called a pulse or wave packet) associated with that dispersion relation. First, for a nonlinear dispersion relation the propagation speed of the pulse will not be equal to the phase velocity. Second, a nonlinear dispersion relation typically leads to the spreading of the pulse with time. (This spreading is also known as dispersion!)

B. Connection to the Coupled Oscillator Problem

So what is the dispersion relation for our coupled oscillator system? By combining Eqs. (11) and (12) we see that we can write

$$\omega(k) = 2\tilde{\omega}\sin\left(\frac{d}{2}k\right) \tag{20}$$

This is another example of a nonlinear dispersion relation.

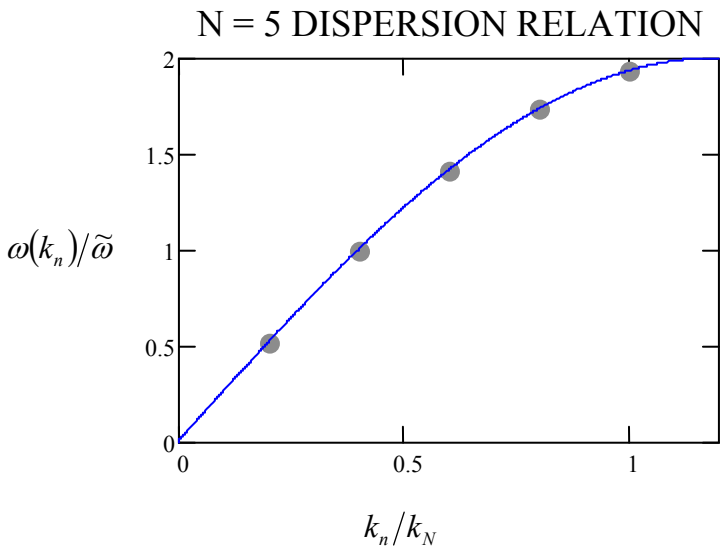
Let's make some graphs of the dispersion relation for the coupled-oscillator system. Now Eq. (20) is correct, but not particularly useful for doing this. That is because for the coupled oscillator problem k can only have the discrete values

$$k_n = \frac{n\pi}{N+1}\frac{1}{d}, \tag{21}$$

where $n = 1, 2, 3, \ldots, N$, are allowed [see Eq. (11)].[5] So we must be a bit clever here. Let's rewrite Eq. (12) as

$$\omega(k_n) = \tilde{\omega}\sin\left(\frac{\pi}{2}\frac{N}{N+1}\frac{n}{N}\right) = 2\tilde{\omega}\sin\left(\frac{\pi}{2}\frac{N}{N+1}\frac{k_n}{k_N}\right). \tag{22}$$

(The rhs follows because $k_n \propto n$. Thus, $n/N = k_n/k_N$.) This makes Eq. (12) look like the dispersion relation that we want, but in constructing a graph, we can simply plot ω vs n/N (keeping in mind that n/N is the same as k_n/k_N.) The following graph plots $\omega(k_n)/\tilde{\omega}$ vs k_n/k_N for $N = 5$.[6]

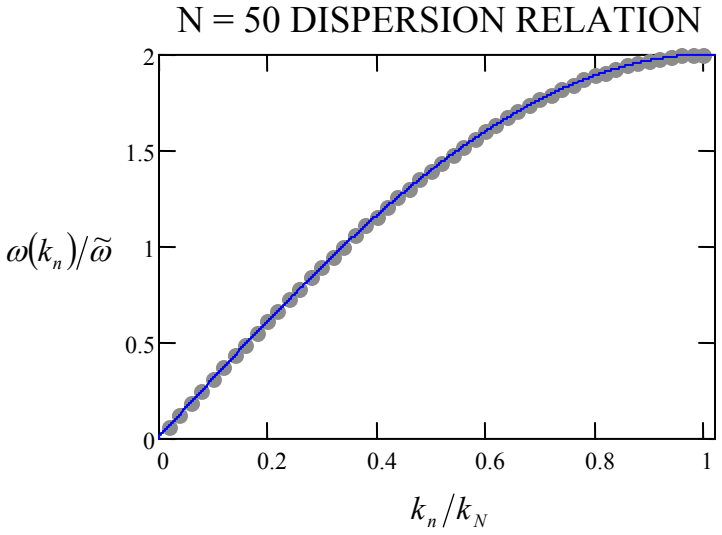


For $N = 5$, k_n is obviously a discrete variable (as the graph shows), but there are times when it is useful (and appropriate) to think of k_n as a continuous variable (even if it

[5] Of course you already knew this because of your familiarity with standing waves on a string (although in that case $N = \infty$ -- more on this later!)

[6] When making a graph, it is often useful to use normalized, unitless quantities for the axes. This makes the graph more widely applicable.

isn't). To see when this is the case, let's consider Eq. (22) for larger N, as illustrated in the next figure, where the dispersion relation is plotted for $N = 50$. The key observation here is that that the spacing between adjacent values of k_n/k_N becomes smaller as N becomes larger. In fact, it is not hard to show that the relative spacing between allowed values of k is given by

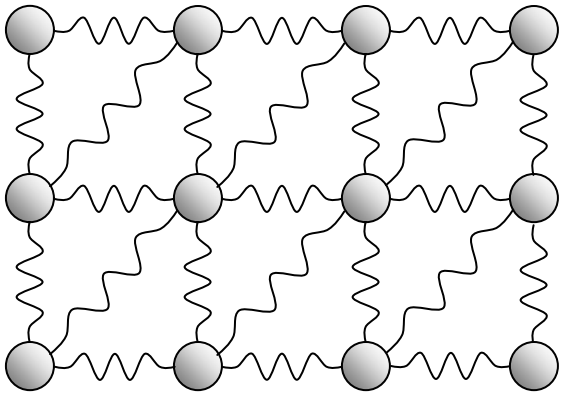


$$\frac{\Delta k}{k_N} = \frac{1}{N}. \tag{20}$$

For very large N, say $N = 10^{23}$ (as one might be interested if one were modeling atoms in a solid as coupled oscillators), the spacing $\Delta k/k_N$ is indeed truly negligible, and one is justified in thinking of k as continuous.

III. Interparticle Interactions and Dispersion Relations

Now you may think that our model of coupled oscillators is nothing more than an exercise in classical mechanics. This model, however, contains the essence of vibrational dynamics in solid-state materials. How can this be? Surely the interactions between atoms in a solid are much more complicated than the quadratic potentials of a bunch of springs. Yes, that is true. However, let's think back to the first lecture where we discussed the Taylor-series expansion of an arbitrary potential energy function near a minimum. We found out that if the object does not stray too far from equilibrium, then the potential is effectively quadratic – that is, the object is pulled back towards equilibrium as if it were attached to a spring. Well, the same thing is true for atoms in a solid. At most temperatures they never stray too far from their

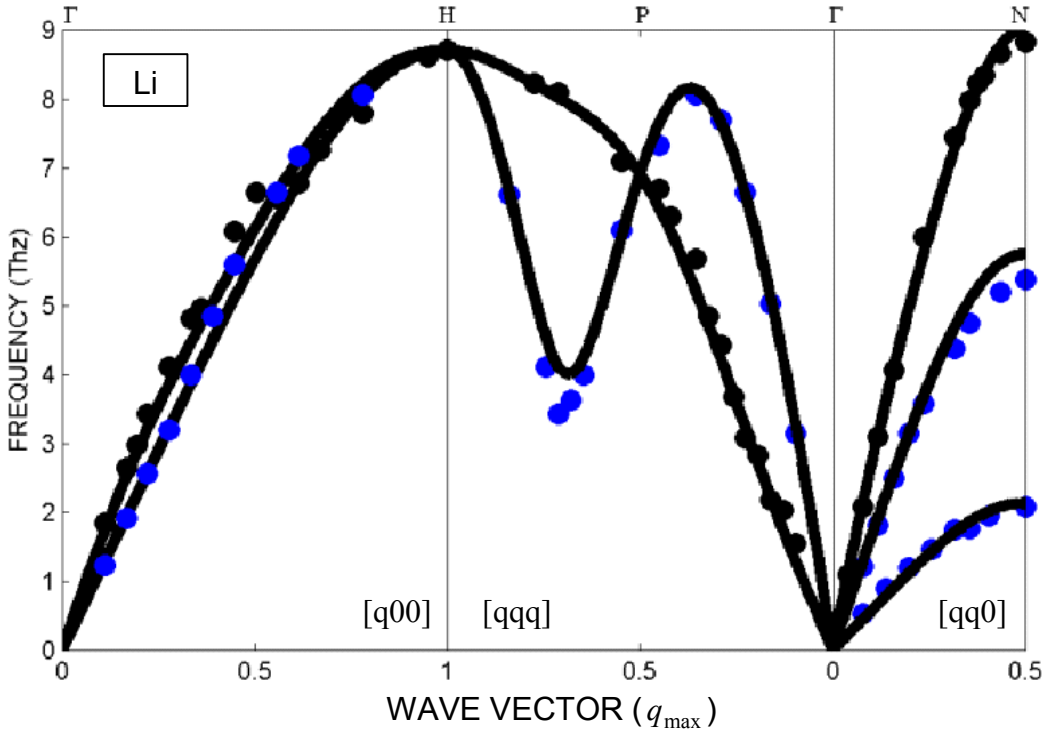


equilibrium positions. What this means is that a model where the atoms are hooked to other atoms with springs is, indeed, a pretty good model. Thus, when thinking of vibrations (i.e., oscillations) of atoms (really, the nuclei because the nucleus contain nearly all the mass of an atom) we can think of the nuclei as if they are attached to other nuclei with springs, as the picture above suggests.

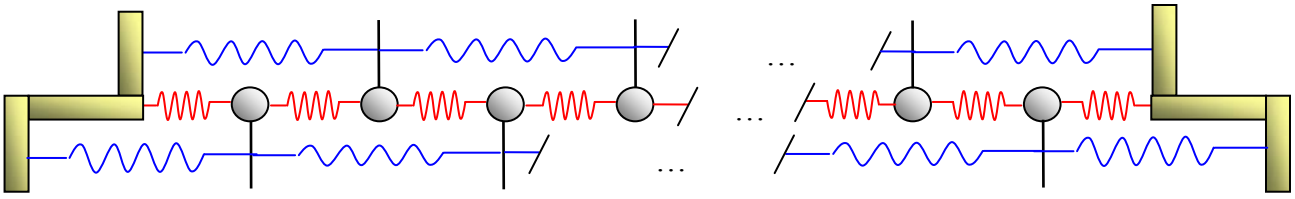
Now because the nuclei are essentially connected together with springs, there is a set of normal modes for the system. Further, as with our case of couple oscillators, there is a dispersion relation associated with the normal modes of vibration. In fact, for every wave vector (which is indeed a vector **k** because of the 3 dimensional nature of the solid) there are three normal modes (because each nucleus can vibrate in three dimensional space).

With regards to solid-state physics, the most important thing about dispersion relations is that they can be measured (and thus compared with theory). The figure on the next page shows both experimental (the discrete points) and calculated (the continuous lines) dispersion curves for Li.

For the wave-vector directions of propagation shown in the graph, there are two normal modes with transverse polarization and one with longitudinal polarization for each value of **k** , although along the (100) and (111) directions the two transverse modes are degenerate (have the same frequency). Notice that along the (100) and (110) directions that the dispersion curves are similar to the dispersion curve for our simple 1D coupled oscillator system. So what is the point? Well, the measured curves provide insight into the microscopic interactions between the atoms: in order to theoretically calculate the dispersion curves one must know which atoms are coupled with springs and what the spring constants are for the different springs.

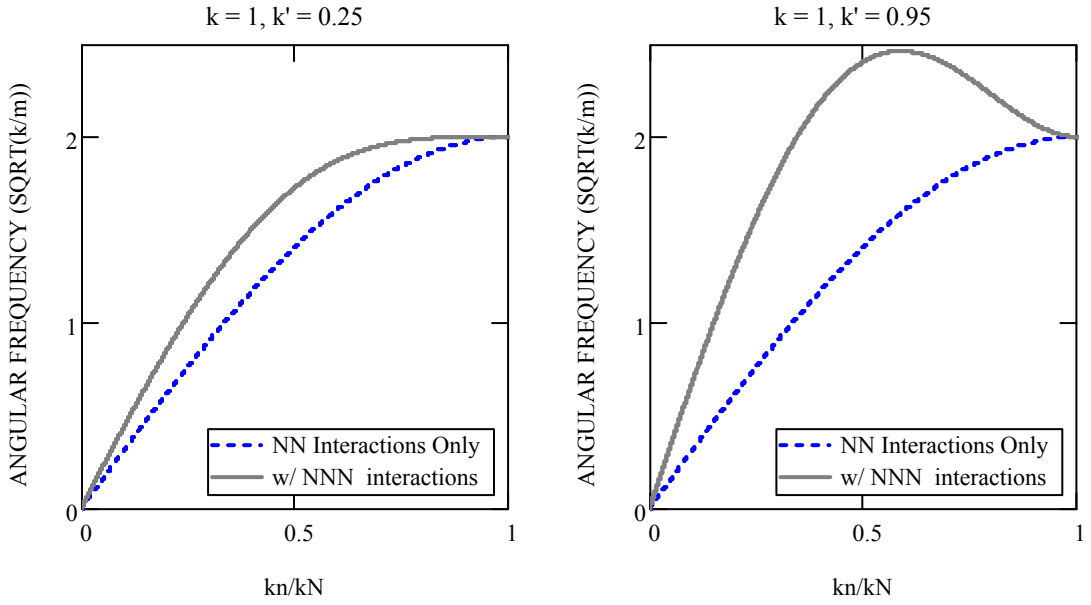


To get a better sense of how the interactions between atoms affect the dispersion curves, let's go back to our simple 1D system and modify it by adding some more springs to see how the dispersion curve is affected. In particular, let's add some next-nearest-neighbor (NNN) springs in addition to the nearest-neighbor (NN) springs that we already have. This modification is illustrated in the following picture.



Of course, so that we have something to play with, we let the NN and NNN springs have different spring constants: we continue to let the NN springs have spring constant k_s while the NNN springs have spring constant k_s'. (Of course, this is what we would expect: why should NN's and NNN's have the same interactions?)

The following picture shows the dispersion curves that result when these NNN springs are added. (These curves are for large N and so are plotted as continuous functions.) Notice that the dispersion curves are quite sensitive to the value of k_s', the spring constant for the NNN interaction. Also notice that the dispersion curve in the graph on the right is similar to the dispersion curve for the longitudinal mode in Li along the (111) direction.



Exercises

*__6.1__ Using the appropriate trig identities, derive Eq. (6) from Eq. (5).

*__6.2__ Under the condition $A_n = B_n = A$, show that Eq. (9) is equivalent to Eq. (8).

*__6.3__ Show that the superposition (sum) of the two standing waves $A\sin(kx)\sin(\omega t)$ and $A\cos(kx)\cos(\omega t)$ is a traveling wave. What is the direction of propagation of this traveling wave?

6.4 **Linear chain with NN and NNN interactions. Here you will find the normal-mode frequencies for a linear chain of coupled oscillators with both NN springs (k) and NNN springs (k').
(**a**) Write down the equation of motion for the j th oscillator for this system. Consulting the picture on p. 9 may be helpful.
(**b**) Analogous to the steps in Sec. II of the Lecture 5 notes, find the normal-mode frequencies Ω_n and show that they can be written as

$$\frac{\Omega_{n\pm}}{\tilde{\omega}} = \pm 2\left[\sin^2\left(\frac{\phi_n}{2}\right) + \left(\frac{\tilde{\omega}'}{\tilde{\omega}}\right)^2 \sin^2(\phi_n)\right]^{1/2}$$

where $\tilde{\omega} = \sqrt{k_s/m}$, $\tilde{\omega}' = \sqrt{k_s'/m}$, and $\phi_n = n\pi/(N+1)$.
(**c**) For this problem plot (using computer software) the dispersion curve $\omega(k_n)/\tilde{\omega}$ vs k_n/k_N for $m = 1$, $k_s = 1$, and $k_s' =$ 0.2, 0.5, and 0.8. You may assume that there are many oscillators so that your dispersion curves are effectively continuous.

*6.5 Show that the spacing between allowed wave vectors for the coupled oscillator problem is given by Eq. (20).

Long Wavelength Limit / Normal Modes

Overview and Motivation: Today we look at the long wavelength limit of the coupled-oscillator system. In this limit the equations of motion for the coupled oscillators can be transformed into the partial differential equation known as the wave equation, which has wide applicability beyond the coupled-oscillator system We also look at the normal modes and the dispersion relation for the coupled-oscillator system in this limit.

Key Mathematics: We again utilize the Taylor-series expansion.

I. Derivation of the Wave Equation

A. The Long Wavelength Limit (LWL)

So why look at the coupled-oscillator system at long wave lengths? Perhaps the main motivation comes from the fact that we are often interested in waves in systems where the wavelength is much longer than the distance between the coupled objects. For example, let's consider audible ($\nu =$ 20 to 20,000 Hz) sound waves in a solid. In a typical solid the speed of sound c is ~2000 m/s, so audible frequencies correspond to wavelengths ($\lambda = c/\nu$) between approximately 0.1 and 100 m. These wavelengths are obviously much greater that the typical interatomic spacing d of 2×10^{-10} m. As we will see, one benefit of the long wavelength limit is that we will no longer need to refer to the displacement of each interacting object: the index j will be "traded in" for the continuous position variable x, so that we will be considering displacements as a function of x and t.

Let's consider the equation of motion for the j th oscillator (which can be any oscillator in the N coupled-oscillator system),

$$\frac{d^2 q_j(t)}{dt^2} = \tilde{\omega}^2 \left[q_{j+1}(t) - 2q_j(t) + q_{j-1}(t) \right]. \tag{1}$$

Let 's go ahead and trade in the discrete object index j for the continuous position variable x via $x = jd$, where d is the equilibrium distance between objects in the chain. Then we can rewrite Eq (1) as

$$\frac{\partial^2 q(x,t)}{\partial t^2} = \tilde{\omega}^2 \left[q(x+d,t) - 2q(x,t) + q(x-d,t) \right]. \tag{2}$$

Notice that the time derivative is now a partial derivative because we are now thinking of the displacement q as a function of two continuous variables, x and t.

Now because d is a small parameter,[1] let's Taylor series expand the two functions $q(x+d,t)$ and $q(x-d,t)$ in a Taylor series in d and $-d$, respectively, about the point x [so in doing this expansion we are thinking about x as some fixed point along the chain and $q(x\pm d,t)$ as a function of $\pm d$]. The two Taylor series are

$$q(x+d,t)=q(x,t)+\frac{\partial q(x,t)}{\partial x}d+\frac{1}{2}\frac{\partial^2 q(x,t)}{\partial x^2}d^2+\ldots \tag{3a}$$

and

$$q(x-d,t)=q(x,t)+\frac{\partial q(x,t)}{\partial x}(-d)+\frac{1}{2}\frac{\partial^2 q(x,t)}{\partial x^2}(-d)^2+\ldots \tag{3b}$$

Keeping all terms up to order d^2 (we consider the validity of this approximation at the end of Sec. II) and substituting Eq. (3) into Eq. (2) gives us

$$\frac{\partial^2 q(x,t)}{\partial t^2}=\tilde{\omega}^2 d^2\frac{\partial q^2(x,t)}{\partial x^2} \tag{4}$$

This is the **wave equation**, which as you can see is a homogeneous, linear, second-order, **partial differential equation**. There is one more thing we need to do, however, in order to make Eq (4) more universally applicable. The term

$$\tilde{\omega}^2 d^2=\frac{k_s}{m}d^2 \tag{5}$$

on the rhs of Eq. (5) is a combination of the fundamental parameters k_s, m, and d of the coupled-oscillator problem. Let's define another constant $c^2=(k_s/m)d^2$ so that we can more generically write the wave equation as

$$\frac{\partial^2 q(x,t)}{\partial t^2}=c^2\frac{\partial q^2(x,t)}{\partial x^2}. \tag{6}$$

[1] Technically, the small parameter in the long wave length limit is the ratio d/λ. Generally, a parameter can only be large or small if it is unitless. Otherwise, whether it is small or large (or somewhere in between) will depend upon the system of units being used.

B. General Applicability of the Wave Equation

The is the standard form of the wave equation that we will use in this class. As we shall see in further study of the wave equation, c is the propagation speed of waves described by Eq. (6).

Now if Eq. (6) were only useful for studying the long wavelength motion of the coupled-oscillator system, it really wouldn't be that interesting. Fortunately, it is applicable in a wide variety of situations, including sound waves in fluids and solids, transverse waves on a string, and electromagnetic waves in vacuum (or other nondispersive media). In each situation the constant c^2 can be related to the underlying physics. For example, for transverse waves on a string, $c^2 = \tau/\mu$, where τ is the tension in the string and μ is the mass per unit length of the string.

II. LWL of Coupled Oscillator Solutions

A. Normal Modes

Let's now look at the coupled-oscillator normal modes in the LWL. As we discussed in Lecture 6, we can write the normal-mode solutions (indexed by n) as a function of x and t as

$$q_{(n)}(x,t) = \sin(k_n x)\left(A_n e^{i\omega(k_n)t} + B_n e^{-i\omega(k_n)t}\right) \tag{7}$$

where the wave vector is given by

$$k_n = \frac{n\pi}{N+1}\frac{1}{d}, \tag{8}$$

and the dispersion relation is

$$\omega(k_n) = 2\tilde{\omega}\sin\left(\frac{d}{2}k_n\right). \tag{9}$$

As written, Eqs. (8) and (9) are expressed in terms of the fundamental (or microscopic) parameters d, $\tilde{\omega}$, and N of the coupled-oscillator problem. Let's see if we can re-express them in terms of c and other more generic (or macroscopic) parameters. Well, the first thing to notice is that the length L of the system (a more generic, macroscopic parameter) can be written in terms of the fundamental parameters N and d as $L = (N+1)d$. The wave vector can thus be simply expressed as

$$k_n = \frac{n\pi}{L}. \tag{10}$$

Well, what about Eq. (9), the dispersion relation? It is not yet clear what to do with $\tilde{\omega}$ in order to obtain a more generic description. This is where the long wavelength limit comes into play again. Recall that the wave vector is related to the wavelength via

$$k_n = \frac{2\pi}{\lambda_n}. \tag{11}$$

This allows us to write Eq. (9) as

$$\omega(\lambda_n) = 2\tilde{\omega}\sin\left(\pi\frac{d}{\lambda_n}\right). \tag{12}$$

Now, the long wavelength limit is exactly the limit $d/\lambda << 1$. Thus, in this limit we can replace the sine function by its (very small) argument, so that Eq. (12) can be expressed as

$$\omega(\lambda_n) = \tilde{\omega}\, d\,\frac{2\pi}{\lambda_n}. \tag{13}$$

And now, using $\tilde{\omega} d = c$ and Eq (11), we have the long-wavelength-limit dispersion relation

$$\omega(k_n) = ck_n. \tag{14}$$

Or, in a more general form that is applicable to any harmonic wave described by the wave equation (not just the normal modes for the coupled-oscillator system where $k = k_n$ is discrete),

$$\omega(k) = ck. \tag{15}$$

So we see that, because c is constant, the dispersion relation for waves described by the wave equation is linear vs k. Looking back at the dispersion curves for the coupled-oscillator system that are plotted in the Lecture 6 notes, you should notice that for small k_n/k_N (which is equivalent to small d/λ_n) that the dispersion curves are indeed linear vs k_n. (The small wave vector limit is thus the same as the long wavelength limit.)

Putting all of this together, we can write the normal modes [Eq. (7)] for long wavelengths as

$$q_{(n)}(x,t) = \sin\left(\frac{n\pi}{L}x\right)\left(A_n e^{ic(n\pi/L)t} + B_n e^{-ic(n\pi/L)t}\right) \tag{16}$$

A remark about the normal modes should be made at this point. The function $\sin(n\pi x/L)$ in Eq. (16) came about because of the boundary conditions, which we can now express as $q(0,t)=0$ and $q(L,t)=0$ [You can check that these boundary conditions are indeed satisfied by $\sin(n\pi x/L)$]. For other boundary conditions we would generally get some linear combination of $\sin(k_n x)$ and $\cos(k_n x)$, and perhaps also different allowed wave vectors k_n (or equivalently, allowed wavelengths λ_n).[2]

B. Neglect of Higher Order Terms in Equation of Motion in the LWL

Now that we have an expression for the normal modes in the LWL, we can check to see that it is OK to neglect the terms in Eq. (3) that are of order higher than d^2. The first thing to notice is that all the odd terms in Eqs. (3a) and (3b) cancel each other when inserted into Eq. (2). Thus we need only consider the even terms. The second thing to notice is that for even m

$$\frac{\partial^m q_{(n)}(x,t)}{\partial x^m} = (-1)^{m/2}\left(\frac{2\pi}{\lambda_n}\right)^m q_{(n)}(x,t). \tag{17}$$

{This is obtainable using Eq. (16) in Eq. (3) [in Eq. (2)]}. Therefore, for example, the ratio of the 4th order term to the 2nd order term, neglecting numerical factors, is given by d^2/λ^2, which is much smaller than 1. Thus, we are justified in neglecting this term (and other higher order terms, which have an even smaller ratio) in Eq. (3), the Taylor series expansion of the equations of motion.

III. The Continuum Limit vs the Long Wavelength Limit

Recall that for N oscillators that there are N normal modes. Well, we have been clever and gotten rid of N in all of our expressions. So what do we do? It depends upon the situation that is being described by the wave equation. As a long wavelength limit of a truly discrete system, one must simply make sure that the waves being described have wavelengths that are much longer that the appropriate interparticle spacing. However, there are times when the wave equation is used, such as in electromagnetism, where there are no underlying oscillators and thus no underlying spacing d to be compared with the wavelength. In those cases, where the wave equation is believed to describe all waves, the long wavelength limit is replaced by a more mathematically technical limit, known as the continuum limit. In this limit one

[2] Think about the normal modes for sound waves in a pipe that is open on both ends vs a pipe with one end open and one end closed. This is explored in Exercise 7.4.

actually takes the limit $d \to 0$. The result is that the terms in Eq. (3) of order greater than d^2 can be neglected exactly. Furthermore, in the limit $d \to 0$ (for fixed L), we see that because $L = (N+1)d$, this limit is equivalent to $N \to \infty$. That is, in the continuum limit the number of normal modes becomes infinite. From here on out, when working with normal modes of the wave equation we will assume that there are, indeed, an infinite number of normal modes. (More details on the continuum limit can be found in Dr. Torre's text, *FWP*.)

Exercises

****7.1 The wave equation for NN and NNN coupled oscillators**

(a) Analogous to Eq, (2), write down the equation of motion for the coupled-oscillator system that has both NN and NNN springs (see the Lecture 6 notes).

(b) Similar to what was done here for the NN system, take the long wavelength limit of this equation of motion and derive the wave equation.

(c) For this system, what is the constant c^2 in terms of the fundamental parameters $\widetilde{\omega}$, $\widetilde{\omega}'$, and d?

***7.2 The long wavelength limit**

(**a**) Derive Eq. (17), which follows from Eq. (16), the expression for the normal mode solutions $q_{(n)}(x,t)$.

(**b**) Given your result in (**a**), Show that the ratio of the d^4 to d^2 terms in the Taylor series expansion of $[q(x+d,t)-2q(x,t)+q(x-d,t)]$, which appears on the rhs of the equation of motion as expressed in Eq. (2), is equal to $-\frac{1}{12}(2\pi)^2(d/\lambda_n)^2$.

(**c**) Thus argue that, compared to the d^2 term, the d^4 term can be neglected in the equation of motion in the LWL.

***7.3** Referring to the Lecture 6 notes, show for large N that the ratio k_n/k_N is equal to $2d/\lambda_n$, thus proving that the long-wavelength and small-wave-vector limits are equivalent.

****7.4 Normal modes for an open-closed pipe**

Consider the following general form for a 1D standing wave,

$$q_S(x,t) = [a\sin(kx) + b\cos(kx)]\sin(\omega t + \phi).$$

(**a**) Show that this is a solution to the wave equation only if ω and k are related by the dispersion relation $\omega = \pm ck$.

(**b**) Let's assume that the normal modes for sound waves in a pipe are of the form $q_S(x,t)$ given above. For a pipe that is open on one end (at $x = 0$) and closed on the

other (at $x = L$) the appropriate boundary conditions are $\frac{\partial q(0,t)}{\partial x} = 0$ and $q(L,t) = 0$. Starting with the above general form of the standing wave solutions $q_S(x,t)$, use the $x = 0$ boundary condition to show that the normal modes of this system have the more specific form

$$q(x,t) = b\cos(kx)\sin(ckt + \phi).$$

(**c**) Further, using the $x = L$ boundary condition, show that the wave vector k can only take on the discrete values $k_n = n\pi/(2L)$ (where $n = 1, 3, 5, \ldots$). [Notice that these wave vectors are not the same as the normal-mode wave vectors for the coupled oscillator problem, given by Eq. (10)]. Thus show that the normal modes of the open-closed pipe can be written as

$$q(x,t) = b\cos\left(\frac{n\pi}{2L}x\right)\sin\left(\frac{n\pi c}{2L}t + \phi\right)$$

(**d**) Thus show that the wavelengths of the normal modes of the open-closed pipe are $\lambda_n = 4L/n$.

1D Wave Equation – General Solution / Gaussian Function

Overview and Motivation: Last time we derived the partial differential equation known as the (one dimensional) wave equation. Today we look at the general solution to that equation. As a specific example of a localized function that can be useful when studying waves, we introduce the Gaussian function.

Key Mathematics: We reacquaint ourselves with the chain rule (for taking derivatives) and look at the Gaussian function and the integral of the Gaussian function, which is known as the error function.

I. Solutions to the Wave Equation

A. General Form of the Solution

Last time we derived the wave equation

$$\frac{\partial^2 q(x,t)}{\partial t^2} = c^2 \frac{\partial^2 q(x,t)}{\partial x^2} \tag{1}$$

from the long wave length limit of the coupled oscillator problem. Recall that c^2 is a (constant) parameter that depends upon the underlying physics of whatever system is being described by the wave equation.

Now it may surprise you, but the solution to Eq. (1) can, quite generally, be written in very succinct form as

$$q(x,t) = f(x+ct) + g(x-ct), \tag{2}$$

where f and g are any "well-behaved" functions. We won't worry about the details of what well-behaved means, but certainly we certainly want their second derivatives to exist. As we previously discussed, $f(x+ct)$ travels in the $-x$ direction at the speed c and $g(x-ct)$ travels in the $+x$ direction at the same speed. To see that Eq. (2) is a solution to Eq. (1) let's calculate the second x and t derivatives of $f(x+ct)$ and $g(x-ct)$. To do this we need the chain rule, which can be written for the case at hand as

$$\frac{\partial h[k(x,t)]}{\partial x} = \frac{dh}{dk}\frac{\partial k}{\partial x} = h'\frac{\partial k}{\partial x}. \tag{3}$$

Applying this rule to $f(x+ct)$, for example, we have

$$\frac{\partial f(x+ct)}{\partial x} = f'(x+ct)\frac{\partial (x+ct)}{\partial x} = f'(x+ct), \tag{4}$$

where $f'(x+ct)$ is the derivative of $f(x+ct)$ with respect to its argument. Applying the chain rule again to calculate the second derivative of $f(x+ct)$ with respect to x give us

$$\frac{\partial^2 f(x+ct)}{\partial x^2} = \frac{\partial f'(x+ct)}{\partial x} = f''(x+ct)\frac{\partial (x+ct)}{\partial x} = f''(x+ct). \tag{5}$$

Similarly, we have for the t derivatives

$$\frac{\partial f(x+ct)}{\partial t} = f'(x+ct)\frac{\partial (x+ct)}{\partial t} = c\, f'(x+ct) \tag{6}$$

and

$$\frac{\partial^2 f(x+ct)}{\partial t^2} = c\frac{\partial f'(x+ct)}{\partial t} = cf''(x+ct)\frac{\partial (x+ct)}{\partial t} = c^2 f''(x+ct). \tag{7}$$

From Eqs. (5) and (7) we see that

$$\frac{\partial^2 f(x+ct)}{\partial t^2} = c^2\frac{\partial^2 f(x+ct)}{\partial x^2} \tag{8}$$

and so $f(x+ct)$ indeed solves the wave equation. Proof that $g(x-ct)$ also satisfies Eq. (1) follows from an essentially identical calculation.

B. More Specific Solutions

So the (totally unknown) functions $f(x+ct)$ and $g(x-ct)$ are solutions, but only in a very general sense. As we shall see, any solution has the form of Eq. (2), but how do we know what the solution will be in any given situation? Well, as with earlier problems that we have looked at in this class, the situation can be specified by **initial conditions** and the **boundary conditions**. Recall, for the coupled oscillator problem the initial conditions were specified by values for $q_j(0)$ and $\dot{q}_j(0)$. Now, however, the spatial variable is not the discrete index j but the continuous variable x. The corresponding initial conditions can thus be written as

$$q(x,0) = a(x) \tag{9a}$$

and

$$\frac{\partial q}{\partial t}(x,0) = b(x), \tag{9b}$$

where $a(x)$ and $b(x)$ are assumed to be known functions. We could have just stuck with $q(x,0)$ and $\frac{\partial q}{\partial t}(x,0)$, but in the long run we save a bit of notational cumbersomeness by using $a(x)$ and $b(x)$ instead. For the coupled-oscillator system the boundary conditions are $q_0(t) = 0$ and $q_{N+1}(t) = 0$. There will be similar instances for the wave equation where we will be interested in waves on a finite sized system. In such cases we will need to specify the condition on $q(x,t)$ at the system boundaries. Indeed, you have already seen an example of this in Exercise 7.4 from the last lecture notes.

II. Initial Value Problem (IVP) for an Infinite System

Here we write the most general solution to the wave equation, given the initial conditions $a(x)$ and $b(x)$. To keep things simple at this point we will assume that the ends of the (1D) system where these waves exist are at $-\infty$ and $+\infty$. In this way we do not have to deal with any boundary conditions. (We will deal with bc's in the next lecture!) From Eq. (2)

$$q(x,t) = f(x+ct) + g(x-ct), \tag{2}$$

we have for $t = 0$

$$a(x) = f(x) + g(x). \tag{10}$$

That is simple enough. What about the other initial condition. Well, taking the t derivative of Eq. (2) and setting it equal to $b(x)$ at $t = 0$ gives us

$$b(x) = c[f'(x) - g'(x)]. \tag{11}$$

Now Eq. (11) can be formally integrated, which gives us

$$\frac{1}{c}\int_{x_0}^{x} b(x')dx' = f(x) - g(x) \tag{12}$$

where x_0 can have any (constant) value. If we now take the sum and difference of Eqs. (10) and (12) we obtain

$$f(x)=\frac{1}{2}\left[a(x)+\frac{1}{c}\int_{x_0}^{x}b(x')dx'\right] \tag{13a}$$

and

$$g(x)=\frac{1}{2}\left[a(x)-\frac{1}{c}\int_{x_0}^{x}b(x')dx'\right] \tag{13b}$$

Using Eq. (13) in Eq. (2) finally gives us the general solution to the initial-value problem

$$q(x,t)=\frac{1}{2}\left[a(x+ct)+a(x-ct)+\frac{1}{c}\int_{x-ct}^{x+ct}b(x')dx'\right]. \tag{14}$$

Notice that the undetermined constant x_0 has disappeared. Eq. (14) is remarkably simple.

II. The Gaussian Function and Two Initial-Value-Problem Examples

A. Gaussian Function

A very useful function in physics is the **Gaussian**, which is defined as

$$G_\sigma(x)=e^{-x^2/\sigma^2}. \tag{15}$$

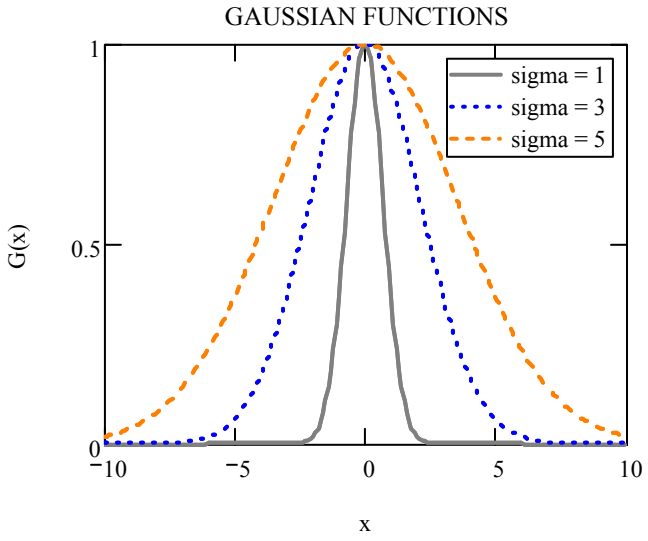
As shown in the picture on the top of the following page, the Gaussian is peaked at $x=0$ and has a width that is proportional to the parameter σ. In fact, the **full width at half maximum** (FWHM), which is the width of the peak at half its maximum height, is equal to $2\sqrt{\ln(2)}\sigma \approx 1.665\sigma$.

B. IVP Solution with Gaussian Initial Position

Let's see what the solution $q(x,t)$ looks like with the initial conditions $a(x)=AG_\sigma(x)$, (A is just some arbitrary amplitude) and $b(x)=0$. (Physically, how would you describe this set of initial conditions?) Using Eq. (14) we rather trivially obtain

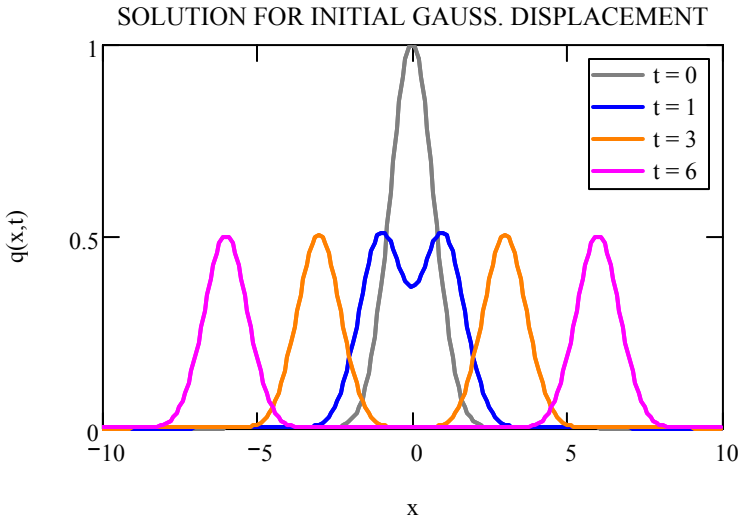
$$q(x,t)=\frac{A}{2}\left[G_\sigma(x+ct)+G_\sigma(x-ct)\right], \tag{16}$$

or more explicitly,



$$q(x,t)=\frac{A}{2}\left[e^{-(x+ct/\sigma)^2}+e^{-(x-ct/\sigma)^2}\right], \tag{17}$$

So the solution consists of two Gaussian functions, one moving in the $-x$ direction and one in the $+x$ direction, both at the speed c. The amplitude of each function is ½ the amplitude of the initial Gaussian displacement. The following picture illustrates this solution as a function of x for several times t. For simplicity we have set $A=1$, $\sigma=1$, and $c=1$.



B. IVP Solution with Gaussian Initial Velocity / Error Function

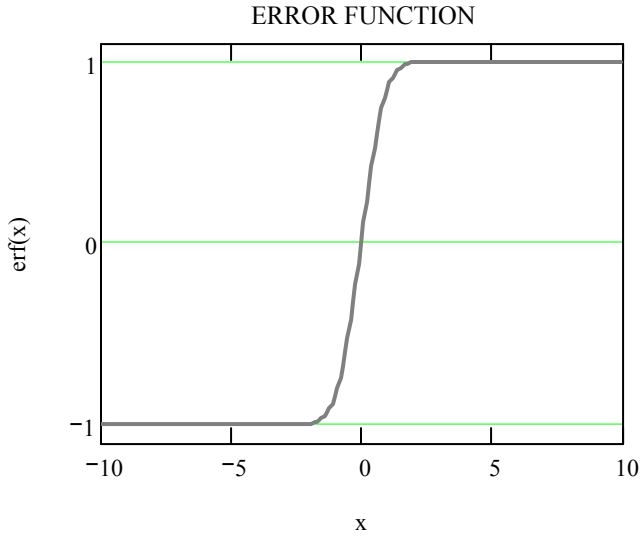
Let's look at another example using the Gaussian function. This time let's have the initial displacement of the system be zero so that $a(x)=0$, but let's have a Gaussian initial-velocity function so that $b(x)=BG_\sigma(x)$, where B is some arbitrary velocity amplitude. In this case we get from Eq. (14)

$$q(x,t)=\frac{B}{2c}\int_{x-ct}^{x+ct} e^{-(x'/\sigma)^2}\,dx'. \tag{18}$$

So what is the integral of a Gaussian function? Well, it is known as the error function. Specifically, the **error function** is defined as

$$erf(x)=\frac{2}{\sqrt{\pi}}\int_0^x e^{-x'^2}\,dx'. \tag{19}$$

The following figure shows a plot of $erf(x)$ vs x. As the graph indicates, $erf(x)$ is defined such that $erf(x\to-\infty)=-1$, $erf(x\to\infty)=1$, and $erf(0)=0$.



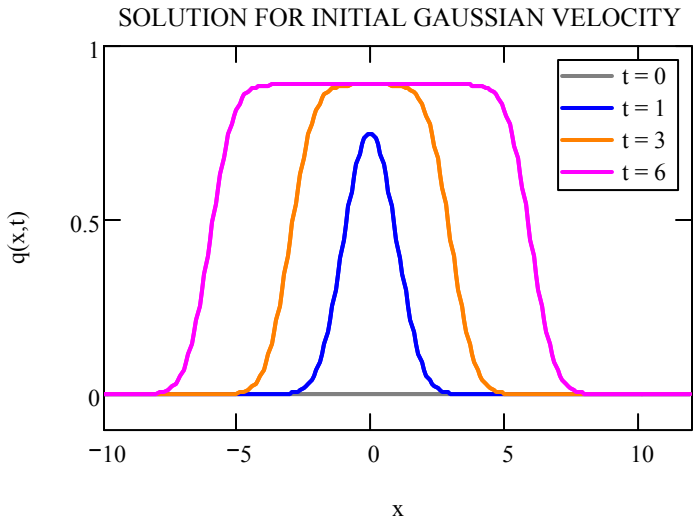
All this is fine and well, but what do we do about the σ in Eq. (18), which does not appear in Eq. (19)? We must do a little math (!) and change variables in Eq. (18). Let's define a new integration variable $y=x'/\sigma$, $dy=dx'/\sigma$. Then Eq. (18) becomes

$$q(x,t)=\frac{B\sigma}{2c}\int_{(x-ct)/\sigma}^{(x+ct)/\sigma} e^{-y^2}\,dy. \tag{20}$$

We can now use Eq. (19), the definition of the error function, to write

$$q(x,t)=\frac{\sqrt{\pi}B\sigma}{4c}\{erf[(x+ct)/\sigma]-erf[(x-ct)/\sigma]\}. \tag{21}$$

Notice that again we have the sum of two functions, each traveling in opposite directions at the speed c. The following picture plots the solution vs x for several values of t (with B, σ, and c all set to 1).



Exercises

*__8.1 The chain rule__. Let $h(x,y)=x^2+xy+y^2$.

(**a**) Directly calculate $\partial h/\partial x$ and $\partial h/\partial y$.

(**b**) Now define two new independent variables $u=(x+y)/2$ and $u=(x-y)/2$

(**c**) Rewrite $h(x,y)$ in terms of u and v. That is, find $h(u,v)$.[1]

(**d**) Now starting with $h(u,v)$ and thinking of it as $h(u(x,t),v(x,t))$, calculate $\partial h/\partial x$ using the chain rule. That is, calculate this derivative using $\frac{\partial h}{\partial x}=\frac{\partial h}{\partial u}\frac{\partial u}{\partial x}+\frac{\partial h}{\partial v}\frac{\partial v}{\partial x}$. Does this agree with your answer in (**a**)?

(**e**) Follow a procedure analogous to that in (**d**) to calculate $\partial h/\partial y$. Again, does this agree with your answer in (**a**)?

[1] Technically speaking, we should give the function $h(u,v)$ another name [$\bar{h}(u,v)$, say], but being physicists, we are rather lazy and typically still call the new function h.

*__8.2__ Verify for $t = 0$ that Eq. (14) and its time derivative reduce to the initial conditions $q(x,0) = a(x)$ and $\frac{\partial q}{\partial t}(x,0) = b(x)$, respectively.

*__8.3__ If the initial displacement is zero, then Eq. (14), the solution to the initial value problem, can be written as $q(x,t) = \frac{1}{2c}\int_{x-ct}^{x+ct} b(x')dx'$. By calculating second derivatives in x and t, directly demonstrate that this function solves Eq. (1), the wave equation.

**__8.4 The error function__.
(**a**) Using an appropriate change of integration variable in the equation $erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-x'^2}dx'$, show that $erf(x/\sigma) = \frac{2}{\sqrt{\pi}\sigma}\int_0^x e^{-(x'/\sigma)^2}dx'$.
(**b**) Using a computer mathematic package, plot $erf(x/\sigma)$ over an appropriate range of x for σ = 1, 3, and 5.

**__8.5 The initial value problem__.
Consider Eq. (14), the general solution to the initial value problem.
(**a**) Explain why Eq. (14) in not a function of the variable x'. (This is a basic feature of the definite integral. Consult a calculus book if necessary.)
(**b**) What are c, $a(x)$, and $b(x)$ in Eq. (14)?
(**c**) Consider the specific case where $a(x) = 0$ and $b(x) = 2cx/(1+x^4)$. Using a computer mathematics package and letting $c = 1$, plot $b(x)$ over an appropriate range of x.
(**d**) Using the initial conditions given in (**c**), solve Eq. (14). (Do not set c to zero!) The integral can be done either with a change of variable, a computer mathematics package, or can be looked up in a table of integrals (such as found in the *CRC Handbook of Chemistry and Physics*).
(**e**) Show that your solution can be written in the form $q(x,t) = f(x+ct) + g(x-ct)$. Thus identify $f(x)$ and $g(x)$.
(**f**) Again, using a computer mathematics package and letting $c = 1$, plot $q(x,t)$ as a function of x for t = 0, 10, 20, and 30. Be careful to let your graph include all interesting parts of the solution!

General Solution with Boundary Conditions

Overview and Motivation: Last time we wrote down the general form of the solution to the 1D wave equation. We then solved the initial-value problem for an infinitely long system. Today we use the same form of the solution and solve the initial-value problem for a finite system with boundary conditions.

Key Mathematics: We again use chain rule for taking derivatives and utilize the Gaussian function.

I. Review of the Initial Value Problem (for an Infinite System)

Last time we considered waves on a one-dimensional system of infinite extent. We wrote down the solution to the wave equation

$$\frac{\partial^2 q(x,t)}{\partial t^2} = c^2 \frac{\partial^2 q(x,t)}{\partial x^2} \tag{1}$$

as

$$q(x,t) = f(x+ct) + g(x-ct), \tag{2}$$

where f and g are any well-behaved functions. In terms of the initial conditions $q(x,0) = a(x)$ and $\partial q(x,0)/\partial t = b(x)$ the functions f and g can be written as

$$f(x) = \frac{1}{2}\left[a(x) + \frac{1}{c}\int_{x_0}^{x} b(x')dx' \right] \tag{3a}$$

and

$$g(x) = \frac{1}{2}\left[a(x) - \frac{1}{c}\int_{x_0}^{x} b(x')dx' \right] \tag{3b}$$

which results in the solution to the initial-value problem

$$q(x,t) = \frac{1}{2}\left[a(x+ct) + a(x-ct) + \frac{1}{c}\int_{x-ct}^{x+ct} b(x')dx' \right]. \tag{4}$$

We then looked at two examples where the initial conditions were related to the Gaussian function.

Today we are going to again consider the initial-value problem, but this time on a system of finite extent, where we will impose some boundary conditions. As we shall see, the bc's impose constraints on the functions $f(x+ct)$ and $g(x-ct)$, with one result being that the motion of the system is periodic.

II. Imposing the Boundary Conditions

Let's assume that the extent of the physical system is from $x=0$ to $x=L$. We consider bc's equivalent to those for the coupled oscillator system

$$q(0,t)=0 \tag{5a}$$

and

$$q(L,t)=0\,. \tag{5b}$$

These bc's are also appropriate for transverse waves on a string where the end supports are fixed or for sound waves that travel along the axis of a pipe that is closed at both ends. For a pipe these bc's are often referred to as closed-closed bc's.

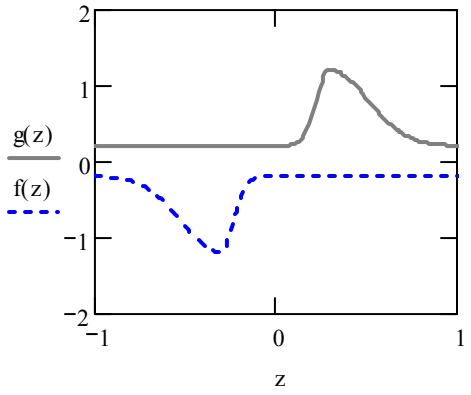
Applying the first bc $q(0,t)=0$ to the form of $q(x,t)$ expressed in Eq. (2) gives us

$$f(ct)=-g(-ct). \tag{6}$$

So what does this equation tell us? Well, because this bc applies for all times t, Eq. (6) is valid for any value of ct, and so we can introduce another variable $z=ct$ and re-express Eq. (6) as

$$f(z)=-g(-z), \tag{7}$$

which must hold for all z. So irrespective of anything else (like the initial conditions), we see that the functions f and g are intimately related. The following picture illustrates the relationship expressed by Eq. (7). The solid curve is (some arbitrary) $g(x)$. The dashed curve is $f(z)$ corresponding to $g(z)$ consistent with Eq. (7).



Let's now consider the second bc $q(L,t)=0$. When applied to Eq. (2) this bc gives

$$f(L+ct)=-g(L-ct). \tag{8}$$

Now, again, because this equation is valid for any value of t, it is valid for any value of ct, so this time let's let $L+ct=z$. Then Eq. (8) can be re-expressed as

$$f(z)=-g(2L-z). \tag{9}$$

And using Eq. (7) to replace $f(z)$ in Eq. (9) gives us

$$g(-z)=g(2L-z), \tag{10}$$

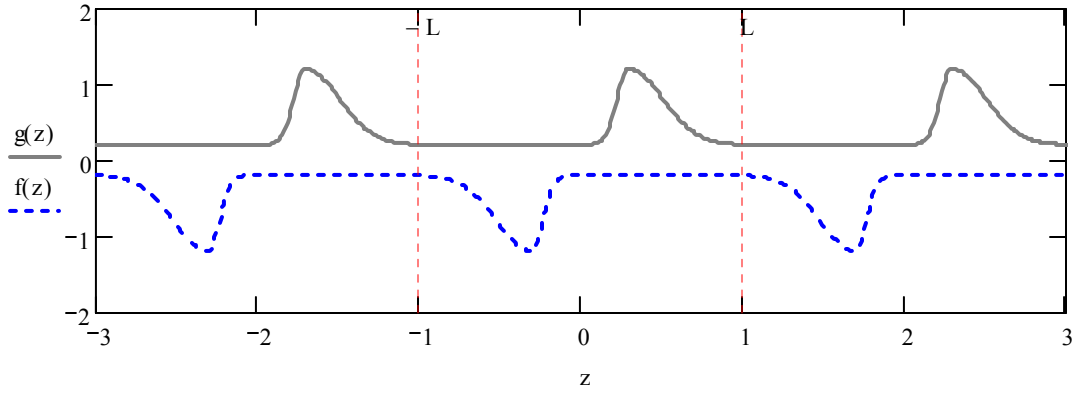
which is valid for all values of z, so let's replace z by $-z$, which results in

$$g(z+2L)=g(z). \tag{11}$$

Now this is very interesting. It says that $g(z)$ is periodic with period $2L$. Of course, because $f(z)=-g(-z)$, $f(z)$ is also periodic with period $2L$. Thus we also have

$$f(z+2L)=f(z). \tag{12}$$

Summarizing, the two bc's $q(0,t)=0$ and $q(L,t)=0$ have imposed the constraints given by Eqs. (7), (11), and (12) on the functions f and g. So our previous illustration of f and g must be modified, as shown in the following picture (where we have set $L=1$).



OK, so something like the following may be bothering you: if f and g are periodic with period $2L$ then, for $t=0$, for example, $f(x+ct)=f(x)$ and $g(x+ct)=g(x)$ are defined outside the physical boundaries of the system, which lies between 0 and L. That is indeed true, but so what? There is no problem in defining f and g as functions of infinite extent; in fact they must be defined over an infinite domain because $f(x+ct)$ and $g(x+ct)$ must be defined for all times t. We just need to remember that they only describe the physical system via $q(x,t)=f(x+ct)+g(x-ct)$ for x between 0 and L.

III. An Initial Value Problem

Let's now look at an initial-value problem with the boundary conditions discussed above. As we did in the last lecture, let's see what happens with an initial Gaussian displacement and no initial velocity, which we write as

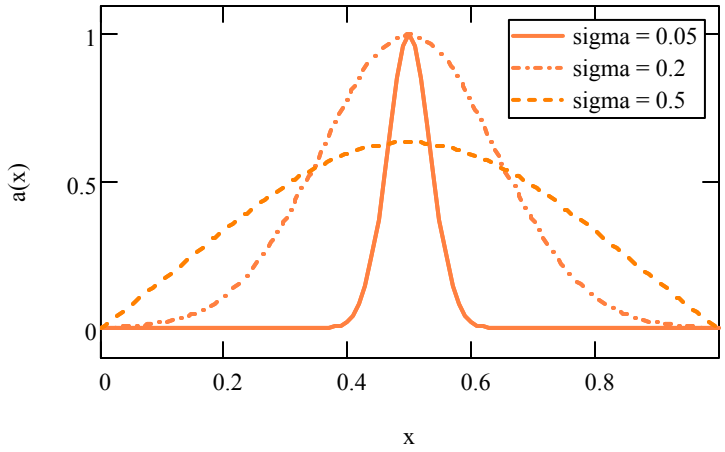
$$a(x)=A\left\{\exp\left[-\left(\frac{x-(L/2)}{\sigma}\right)^2\right]-\exp\left[-\left(\frac{(L/2)}{\sigma}\right)^2\right]\right\} \tag{13a}$$

and

$$b(x)=0\,. \tag{13b}$$

If you compare Eq. (13a) to the similar initial condition that we discussed in Lecture 9, you will notice that it is slightly more complicated. First, the Gaussian function is centered at $x=L/2$ rather than $x=0$. Second, we have subtracted off a constant from the Gaussian: this insures that the two bc's are satisfied by the initial condition. This particular initial condition is illustrated in the next picture for three values of σ,

$\sigma = 0.05$, $\sigma = 0.2$, and $\sigma = 0.5$. ($A = 1$ and $L = 1$ for both initial conditions). We must also keep in mind that outside the interval $0 < x < 1$, $a(x)$ and $b(x)$ are not defined.



Let's see what this initial condition tells us about the functions f and g. Referring to Eq. (3) we see that

$$f(x) = g(x) = \frac{1}{2}a(x), \tag{14}$$

but because $a(x)$ is only defined on the interval $0 \le x \le L$, this equation is only valid in that domain. We must use Eqs. (7), (11), and (12) to define $f(x)$ and $g(x)$ outside this domain. Using Eq. (7) we can define both functions for $-L \le x < 0$. Eq. (7) and Eq. (14) together imply

$$f(-x) = -f(x), \tag{15a}$$

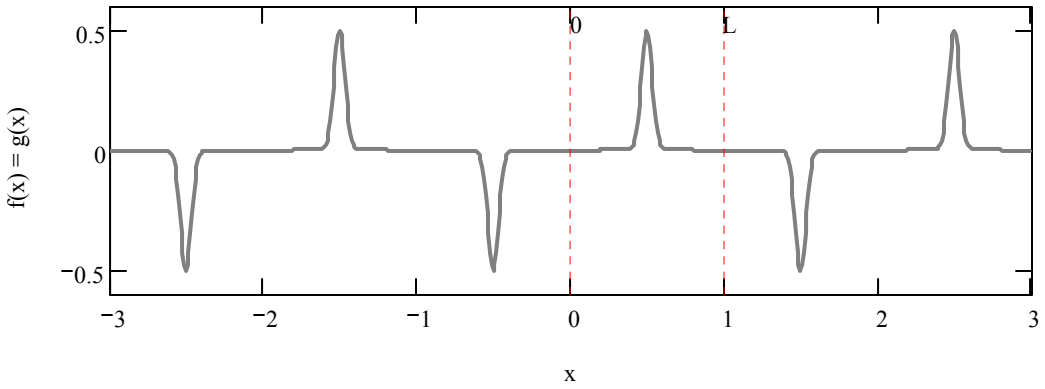
and

$$g(-x) = -g(x). \tag{15b}$$

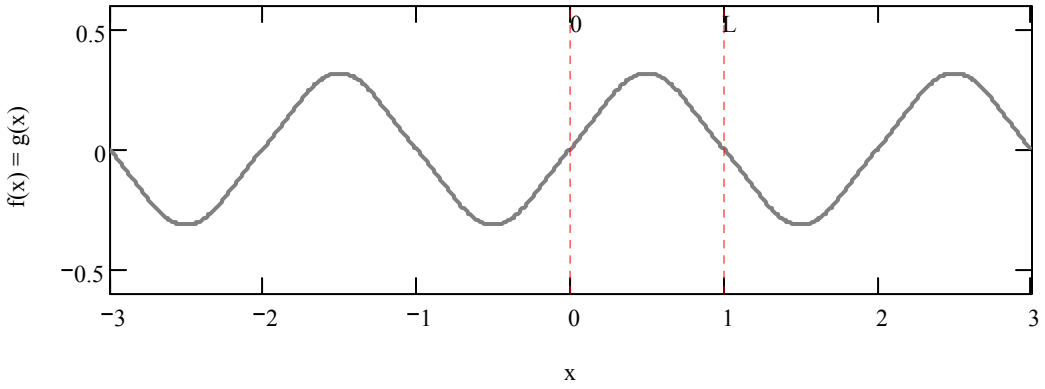
That is, $f(x)$ and $g(x)$ are both odd about $x = 0$. We now know what $f(x)$ and $g(x)$ are for $-L \le x < L$. We can use Eqs. (11) and (12), which tell us that both functions are periodic with period $2L$, to define $f(x)$ and $g(x)$ outside this interval. Putting all of this together, we can formally write the functions $f(x)$ and $g(x)$ as

$$f(x)=g(x)=\frac{1}{2}\sum_{m=-\infty}^{\infty}\left[a(x-2mL)-a(-x+2mL)\right], \tag{16}$$

but we must remember that $a(x)$ is only defined on the interval $0<x<L$.
For the initial condition described by Eq. (13) with $a_0=0.05$, the following figure plots $f(x)=g(x)$.



So now that we know $f(x)$ and $g(x)$ for all values of their arguments, we have the solution to the initial value problem via Eq. (2). Instead of a picture to illustrate the time-dependent motion, go check out Video 1 for Lecture 9 on the class web site.[1] Notice that $f(x)$ and $g(x)$ are indeed constructed so that the bc's are satisfied. Also notice that the effect of the bc's is to make the Gaussian pulses flip over when they reflect from the boundaries. Further, notice that the motion is indeed periodic in time. Can you figure out what the period is?



[1] In the video the functions f and g have been displaced vertically for clarity.

Let's also look at the case of the initial condition with $\sigma = 0.5$, illustrated on p. 5? The picture at the bottom of the preceding page plots $f(x) = g(x)$ for this case. These functions look similar to harmonic functions, but they are not – they too are described by Eq. (13). As you can see in Video 2 for Lecture 9, the resulting motion is similar to an harmonic standing wave.

Summarizing, we have seen that in a finite system with boundary condition, the solution to the wave equation can again be written in the form of Eq. (2), the sum of waves traveling at speed c and propagating in the $-x$ and $+x$ directions. The boundary conditions, however, put constraints on the traveling-wave functions f and g. These constraints, in turn, make the motion of the system periodic.

Exercises

***9.1** Show that Eq. (13a) satisfies the bc's [Eq. (5a) and (5b)] for the problem discussed in the notes.

***9.2** For the problem discussed in the notes (waves on a string located between $x = 0$ and $x = L$) find the temporal period of the motion in terms of the parameters c and L.

****9.3** Because $q(x,t) = Ae^{-(x-ct)^2/\sigma^2}$ is a function of $x - ct$, it is a solution to the wave equation (on an infinite domain).
(**a**) What are the initial conditions [$a(x)$ and $b(x)$] that give rise to this form of $q(x,t)$?
(**b**) If $f(x)$ is constant, then Eq. (2) shows that solution is only a function of $x - ct$. For the condition that $f(x)$ is constant find $b(x)$ in terms of $a(x)$. [Hint: consider Eq. (3a).]
(**c**) Show that the initial conditions you found in part (**a**) satisfy the relationship that you found in part (**b**).

General Solution using Normal Modes

Overview and Motivation: Last time we solved the initial-value problem (IVP) for the 1D wave equation on a finite domain with "closed-closed" bc's using the general form of the solution $q(x,t) = f(x+ct) + g(x-ct)$. Today we solve the same problem using the normal mode solutions for this system.

Key Mathematics: We utilize some integrations involving harmonic functions.

I. The Problem Defined

We are looking for the general solution to the wave equation

$$\frac{\partial^2 q(x,t)}{\partial t^2} = c^2 \frac{\partial^2 q(x,t)}{\partial x^2} \tag{1}$$

on the finite domain $0 \le x \le L$ subject to the initial conditions

$$q(x,0) = a(x) \text{ and } \frac{\partial q}{\partial t}(x,0) = b(x) \tag{2a), (2b)}$$

and the boundary conditions

$$q(0,t) = 0 \text{ and } q(L,t) = 0\,. \tag{3a), (3b)}$$

This time we write the solution $q(x,t)$ as linear combination[1] of the normal-mode solutions $q_n(x,t)$

$$q(x,t) = \sum_{n=1}^{\infty} q_{(n)}(x,t), \tag{4}$$

where the normal modes can be expressed as

$$q_{(n)}(x,t) = \sin(k_n x)\left(A_n e^{i\omega_n t} + B_n e^{-i\omega_n t}\right). \tag{5}$$

Here $k_n = n\pi/L$ is the wave vector and $\omega_n = ck_n$ is the angular frequency. As before, let's make the normal-mode solutions explicitly real by setting $B_n = A_n^*$. Then Eq. (5) can be written as

[1] As written, Eq. (4) looks like a simple sum, not a linear combination, but as Eq. (5) shows, we have kept undetermined amplitudes as part of our normal modes, so Eq. (4) may be justifiably thought of as a linear combination of normal modes.

$$q_{(n)}(x,t) = \sin(k_n x)\left[\mathrm{Re}(a_n)\cos(\omega_n t) - \mathrm{Im}(a_n)\sin(\omega_n t)\right], \tag{6}$$

where we have defined a new amplitude $a_n = A_n/2$. Using Eq. (6) we may thus express the general solution [via Eq. (4)] as

$$q(x,t) = \sum_{n=1}^{\infty} \sin(k_n x)\left[\mathrm{Re}(a_n)\cos(\omega_n t) - \mathrm{Im}(a_n)\sin(\omega_n t)\right], \tag{7}$$

As we shall shortly see, the amplitudes a_n are determined by the initial conditions. Recall, however, that normal modes already satisfy the bc's, and so the general solution as expressed by Eq. (7) automatically satisfies those bc's. We thus need not consider the bc's any further.

II. The Initial Value Problem (Yet Again!)

Let's now apply the initial conditions and see what we get. From Eq. (7) we obtain for the initial displacement

$$a(x) = \sum_{n=1}^{\infty} \sin\left(\tfrac{n\pi}{L}x\right)\mathrm{Re}(a_n), \tag{8}$$

and for the initial velocity, we obtain after differentiating Eq. (7)

$$b(x) = \sum_{n=1}^{\infty} -\omega_n \sin\left(\tfrac{n\pi}{L}x\right)\mathrm{Im}(a_n). \tag{9}$$

In Eqs. (8) and (9) we have used $k_n = n\pi/L$. So what do we have here? Well, perhaps not surprisingly, we have two equations for the amplitudes a_n in terms of the initial conditions. However, unlike the (finite) *N*-oscillator case, the rhs's of Eqs. (8) and (9) have an infinite number of amplitudes because the wave equation has an infinite number of normal modes!

Aside: The N -oscillator problem

This looks pretty grim, but perhaps a look back at the *N*-oscillator case will give us some insight into the current problem. For the *N* oscillator problem the equation equivalent to Eq. (8) is the extension of Eq. (19) from the Lecture (6) notes to *N* oscillators, which we can write as

$$\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \\ \vdots \\ q_N(0) \end{pmatrix} = \sum_{n=1}^{N} \begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix} \mathrm{Re}(a_n), \tag{10}$$

where we have again made the assignment $a_n = A_n/2$. Now recall what we did there. To find any particular amplitude $\mathrm{Re}(a_m)$ (which we label by m) we take the m th eigenvector expressed as a row vector and multiply Eq. (10) by that vector. We can write this multiplication as

$$\left(\sin\left(\frac{m\pi}{N+1}1\right) \;\; \sin\left(\frac{m\pi}{N+1}2\right) \;\; \sin\left(\frac{m\pi}{N+1}3\right) \;\; \ldots \;\; \sin\left(\frac{m\pi}{N+1}N\right)\right)\left[\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \\ \vdots \\ q_N(0) \end{pmatrix} = \sum_{n=1}^{N} \begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix} \mathrm{Re}(a_n)\right], \tag{11}$$

Now recall what happens in that case: when the rhs is multiplied by the m th eigenvector, the only term in the sum that survives in the sum is the on with the same eigenvector. That is, only the $n = m$ term survives, which transforms Eq. (11) into

$$\left(\sin\left(\frac{m\pi}{N+1}1\right) \;\; \sin\left(\frac{m\pi}{N+1}2\right) \;\; \sin\left(\frac{m\pi}{N+1}3\right) \;\; \ldots \;\; \sin\left(\frac{m\pi}{N+1}N\right)\right)\left[\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \\ \vdots \\ q_N(0) \end{pmatrix} = \begin{pmatrix} \sin\left(\frac{m\pi}{N+1}1\right) \\ \sin\left(\frac{m\pi}{N+1}2\right) \\ \sin\left(\frac{m\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{m\pi}{N+1}N\right) \end{pmatrix} \mathrm{Re}(a_m)\right], \tag{12}$$

Notice that this equation only has one coefficient $\mathrm{Re}(a_m)$on the rhs and so it can now be solved for that coefficient,

$$\mathrm{Re}(a_m) = \frac{\begin{pmatrix}\sin\left(\frac{m\pi}{N+1}1\right) & \sin\left(\frac{m\pi}{N+1}2\right) & \sin\left(\frac{m\pi}{N+1}3\right) & \ldots & \sin\left(\frac{m\pi}{N+1}N\right)\end{pmatrix}\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \\ \vdots \\ q_N(0)\end{pmatrix}}{\begin{pmatrix}\sin\left(\frac{m\pi}{N+1}1\right) & \sin\left(\frac{m\pi}{N+1}2\right) & \sin\left(\frac{m\pi}{N+1}3\right) & \ldots & \sin\left(\frac{m\pi}{N+1}N\right)\end{pmatrix}\begin{pmatrix}\sin\left(\frac{m\pi}{N+1}1\right) \\ \sin\left(\frac{m\pi}{N+1}2\right) \\ \sin\left(\frac{m\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{m\pi}{N+1}N\right)\end{pmatrix}}. \tag{13}$$

The key point here is that multiplying Eq. (10) by the m th eigenvector allows us to find $\mathrm{Re}(a_m)$ in terms of the initial condition on the displacement of the system. Notice that Eq. (10) is an equation for the initial displacement of the system in terms of the set of coefficients $\mathrm{Re}(a_n)$, while Eq. (13) is an equation for any coefficient $\mathrm{Re}(a_m)$ (labeled by m) in terms of the initial displacement of the system. We can thus think of Eq. (13) as the **inversion** of Eq. (10).

Now the notation used in Eqs. (10) – (13) is rather cumbersome. Fortunately there is a more succinct way to express these equations. Looking at Eq. (10) we first note that the j th element of that equation can be written as

$$q_j(0) = \sum_{n-1}^{N} \sin\left(\frac{n\pi}{N+1}j\right)\mathrm{Re}(a_n). \tag{14}$$

We now notice that if we multiply this equation by $\sin\left(\frac{m\pi}{N+1}j\right)$ and them sum the equation on j,

$$\sum_{j=1}^{N} \sin\left(\frac{m\pi}{N+1}j\right) q_j(0) = \sum_{j=1}^{N} \sin\left(\frac{m\pi}{N+1}j\right) \sum_{n=1}^{N} \sin\left(\frac{n\pi}{N+1}j\right)\, \mathrm{Re}(a_n), \tag{15}$$

then this is indeed multiplication of Eq. (10) by the transpose of the m th eigenvector! That is, Eq. (15) is the same equation as Eq. (11), only in a much more succinct form. We now switch the order of the sums on the rhs

$$\sum_{j=1}^{N} \sin\left(\frac{m\pi}{N+1}j\right) q_j(0) = \sum_{n=1}^{N} \mathrm{Re}(a_n) \sum_{j=1}^{N} \sin\left(\frac{m\pi}{N+1}j\right)\sin\left(\frac{n\pi}{N+1}j\right) \tag{16}$$

and notice that the sum on j on the rhs is simply the product of the (transpose of) m th eigenvector with the n th eigenvector, which is nonzero only if they are the same eigenvector. That is, the sum on j on the rhs is nonzero only if $n = m$. Thus Eq. (16) simplifies to

$$\sum_{j=1}^{N} \sin\left(\tfrac{m\pi}{N+1} j\right) q_j(0) = \mathrm{Re}(a_m) \sum_{j=1}^{N} \sin^2\left(\tfrac{m\pi}{N+1} j\right) . \tag{17}$$

This is equivalent to Eq. (12), only in much more elegant notation. As with Eq. (12) we now only have one amplitude, $\mathrm{Re}(a_m)$, on the rhs. We can thus solve Eq. (12) for this amplitude, obtaining

$$\mathrm{Re}(a_m) = \frac{\sum_{j=1}^{N} \sin\left(\tfrac{m\pi}{N+1} j\right) q_j(0)}{\sum_{j=1}^{N} \sin^2\left(\tfrac{m\pi}{N+1} j\right)}, \tag{18}$$

[which is equivalent to Eq. (13)].

Back to the wave-equation IVP

So how does this apply to the current problem? Well, the main difference between the two problems is that x is a continuous variable while j is discrete. But if we remember a bit of calculus, we should recall that an integral is really just a sum over a continuous variable. We thus might expect the sums over j in Eq. (15) to be replaced by integrals over x. Let's try it and wee what happens. Multiplying Eq. (8) by $\sin\left(\tfrac{m\pi}{L} x\right)$ and integrating on x from 0 to L gives us

$$\int_0^L \sin\left(\tfrac{m\pi}{L} x\right) a(x)\, dx = \int_0^L \sin\left(\tfrac{m\pi}{L} x\right) \sum_{n=1}^{\infty} \sin\left(\tfrac{n\pi}{L} x\right) \mathrm{Re}(a_n)\, dx , \tag{19}$$

and switching the order of integration and summation on the rhs produces

$$\int_0^L \sin\left(\tfrac{m\pi}{L} x\right) a(x)\, dx = \sum_{n=1}^{\infty} \mathrm{Re}(a_n) \int_0^L \sin\left(\tfrac{m\pi}{L} x\right) \sin\left(\tfrac{n\pi}{L} x\right) dx , \tag{20}$$

the continuous-variable analog to Eq. (16). Further, analogous to what happened with the sum on j on the rhs of Eq (16), the integral on the rhs of Eq. (20) is nonzero only if $n = m$. Thus Eq. (20) simplifies to

$$\int_0^L \sin\left(\tfrac{m\pi}{L}x\right)a(x)\,dx = \mathrm{Re}(a_m)\int_0^L \sin^2\left(\tfrac{m\pi}{L}x\right)dx, \tag{21}$$

and so, as above, we can solve for $\mathrm{Re}(a_m)$

$$\mathrm{Re}(a_m) = \frac{\displaystyle\int_0^L \sin\left(\tfrac{m\pi}{L}x\right)a(x)\,dx}{\displaystyle\int_0^L \sin^2\left(\tfrac{m\pi}{L}x\right)dx}, \tag{22}$$

Notice the striking similarity between Eqs. (22) and (18) [especially when you recall that $a(x) = q(x,0)$]. Now, we can simplify Eq. (22) even a bit more. Using the fact that

$$\int_0^L \sin^2\left(\tfrac{m\pi}{L}x\right)dx = \frac{L}{2} \tag{23}$$

we have the result

$$\mathrm{Re}(a_m) = \frac{2}{L}\int_0^L \sin\left(\tfrac{m\pi}{L}x\right)a(x)\,dx. \tag{24}$$

So we now have $\mathrm{Re}(a_m)$ expressed in terms of the initial displacement $a(x)$. Similarly, the imaginary part of a_m can be expressed in terms of the initial velocity $b(x)$ as

$$\mathrm{Im}(a_m) = -\frac{2}{L\omega_m}\int_0^L \sin\left(\tfrac{m\pi}{L}x\right)b(x)\,dx, \tag{25}$$

As mentioned above when discussing the N-oscillator problem, you should think of Eqs. (24) and (25) as the inversions of Eqs. (8) and (9), respectively. Also note, there is nothing special about the index m in these last two equations. We could used any variable. In particular, when thought of as the inversion of Eqs. (8) and (9) we

normally use the variable n to label the amplitudes and write these last two equations as

$$\mathrm{Re}(a_n) = \frac{2}{L}\int_0^L \sin\left(\tfrac{n\pi}{L}x\right) a(x)\, dx\,. \tag{26}$$

and

$$\mathrm{Im}(a_n) = -\frac{2}{L\omega_n}\int_0^L \sin\left(\tfrac{n\pi}{L}x\right) b(x)\, dx\,. \tag{27}$$

Summarizing, Eq. (7), which can be written as

$$q(x,t) = \sum_{n=1}^{\infty} \sin\left(\tfrac{n\pi}{L}x\right)\left[\mathrm{Re}(a_n)\cos\left(c\tfrac{n\pi}{L}t\right) - \mathrm{Im}(a_n)\sin\left(c\tfrac{n\pi}{L}t\right)\right], \tag{28}$$

along with Eqs. (26) and (27) are the complete solution to the initial value problem on the finite domain $0 \le x \le L$ for the bc's $q(0,t) = 0$ and $q(L,t) = 0$.

III. An Example Revisited

Let's consider the problem that we solved in the Lecture 9 Notes. Looking at this problem again will give us a good comparison of the two methods of solving the initial value problem.

The problem in the Lecture 9 notes has the initial conditions[2]

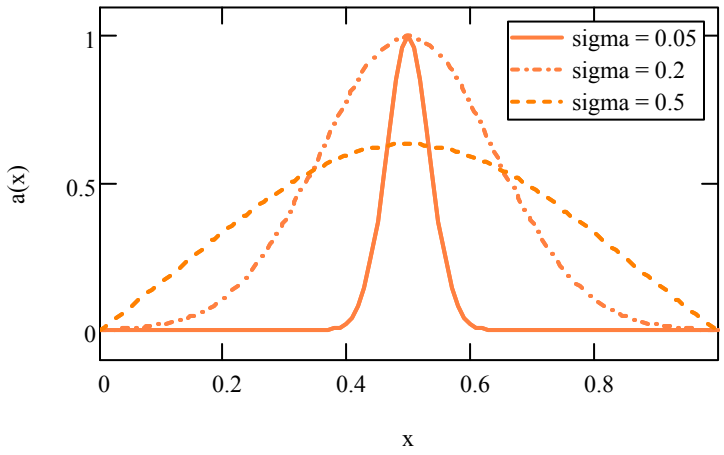
$$a(x) = A\left\{\exp\left[-\left(\frac{x-(L/2)}{\sigma}\right)^2\right] - \exp\left[-\left(\frac{(L/2)}{\sigma}\right)^2\right]\right\} \tag{29a}$$

and

$$b(x) = 0\,. \tag{29b}$$

[2] OK, so we now have another amplitude A, but it is not the same as the amplitudes A_n ($n = 1, 2, \ldots$) used earlier in Eq. (5).

Recall that $a(x)$ is a Gaussian peak that is (vertically) shifted so that the bc's are satisfied. The following figure plots $a(x)$ for the same values of the width parameter σ that we investigated in Lecture 9: $\sigma = 0.05$, $\sigma = 0.2$, and $\sigma = 0.5$.



The easy part of this particular problem is solving for $\mathrm{Im}(a_n)$. Using Eq. (27) we immediately see that $\mathrm{Im}(a_n) = 0$. Similarly (but not as simply!), using Eq. (26) we see that $\mathrm{Re}(a_n)$ is given by

$$\mathrm{Re}(a_n) = \frac{2A}{L}\int_0^L \sin\left(\tfrac{n\pi}{L}x\right)\left\{\exp\left[-\left(\tfrac{x-(L/2)}{\sigma}\right)^2\right] - \exp\left[-\left(\tfrac{L/2}{\sigma}\right)^2\right]\right\} dx. \tag{30}$$

Unfortunately, the integral in Eq. (30) has no analytic solution.[3] Fortunately, a program such as Mathcad can numerically solve the integral. Unfortunately, as Eq. (28) indicates, we need an infinite number of a_n's! Fortunately, in most cases we only need to use a finite number of the a_n's in order to get a very good approximation to the exact solution. That is, in practice we typically use a truncated version of Eq. (28), which we can write as

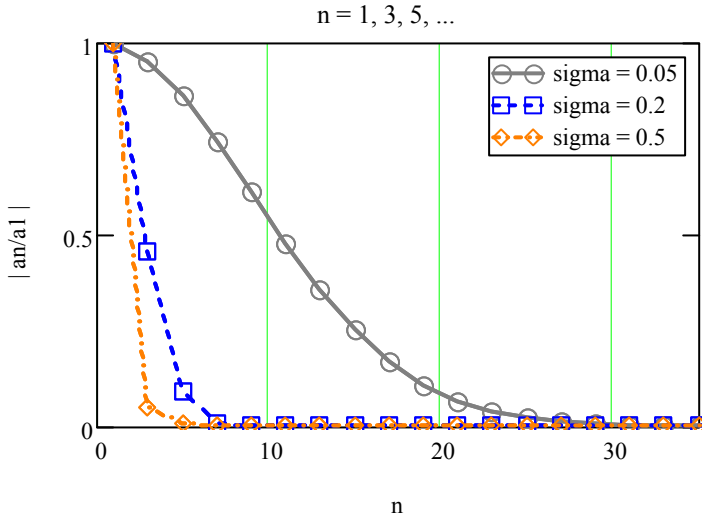
$$q(x,t)_M = \sum_{n=1}^{M} \sin\left(\tfrac{n\pi}{L}x\right)\left[\mathrm{Re}(a_n)\cos\left(c\tfrac{n\pi}{L}t\right) - \mathrm{Im}(a_n)\sin\left(c\tfrac{n\pi}{L}t\right)\right], \tag{31}$$

where $q(x,t)_M$ is the M-term approximation to $q(x,t)$. For the example at hand $\mathrm{Im}(a_n) = 0$ so we have

[3] At least as far as I know! Actually, it is not too difficult to show that $a_n = 0$ if n is even. But that still leaves the odd values of n to deal with.

$$q(x,t)_M = \sum_{n=1}^{M} \sin\left(\tfrac{n\pi}{L}x\right)\mathrm{Re}(a_n)\cos\left(c\tfrac{n\pi}{L}t\right), \tag{32}$$

So how many terms do we need to use? The answer, of course depends upon the accuracy that we require. But we can get a pretty good idea of the number of terms



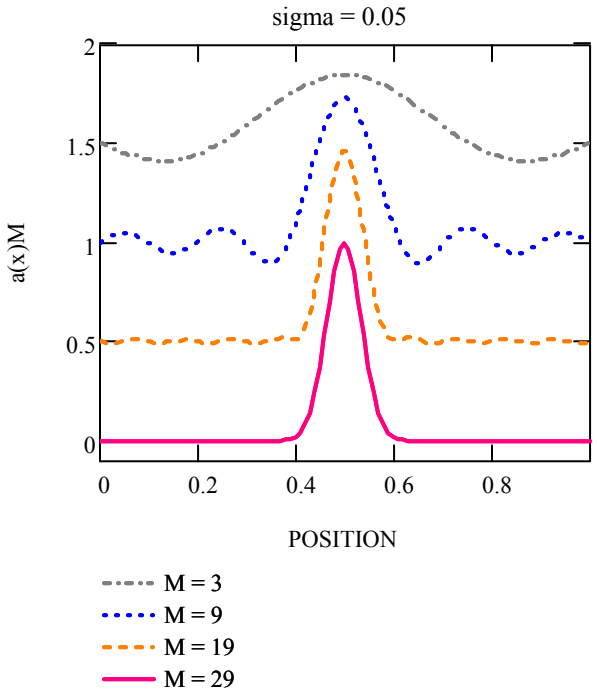
needed by plotting the absolute value of a_n vs n, as shown in the graph on the previous page. The three curves correspond to the three values of σ used in the previous graph. Note that the y-axis values have been normalized by $|a_1|$. Also, because $a_n = 0$ for even n, we have only plotted a_n for odd values of n.

Now this graph is very interesting: it shows that the more compact or sharper the wave (as indicated, in this case by a smaller value of σ), the more normal modes one must use to accurately describe the wave. From the above graph we see that for $\sigma = 0.05$, we need to use $M \approx 29$ to well-represent the wave, for $\sigma = 0.2$ we need $M \approx 5$, and for $\sigma = 0.5$ we need $M \approx 3$.

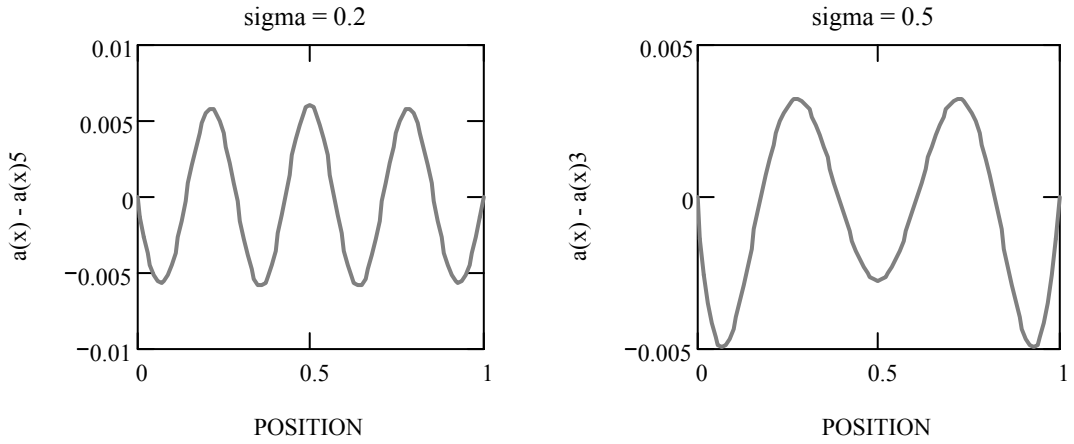
We can also ascertain the number of normal modes needed by comparing the initial condition $a(x)$ with the approximation $q(x,t)_M$ at $t = 0$. At $t = 0$ Eq. (32) becomes

$$a(x)_M = \sum_{n=1}^{M} \sin\left(\tfrac{n\pi}{L}x\right)\mathrm{Re}(a_n), \tag{33}$$

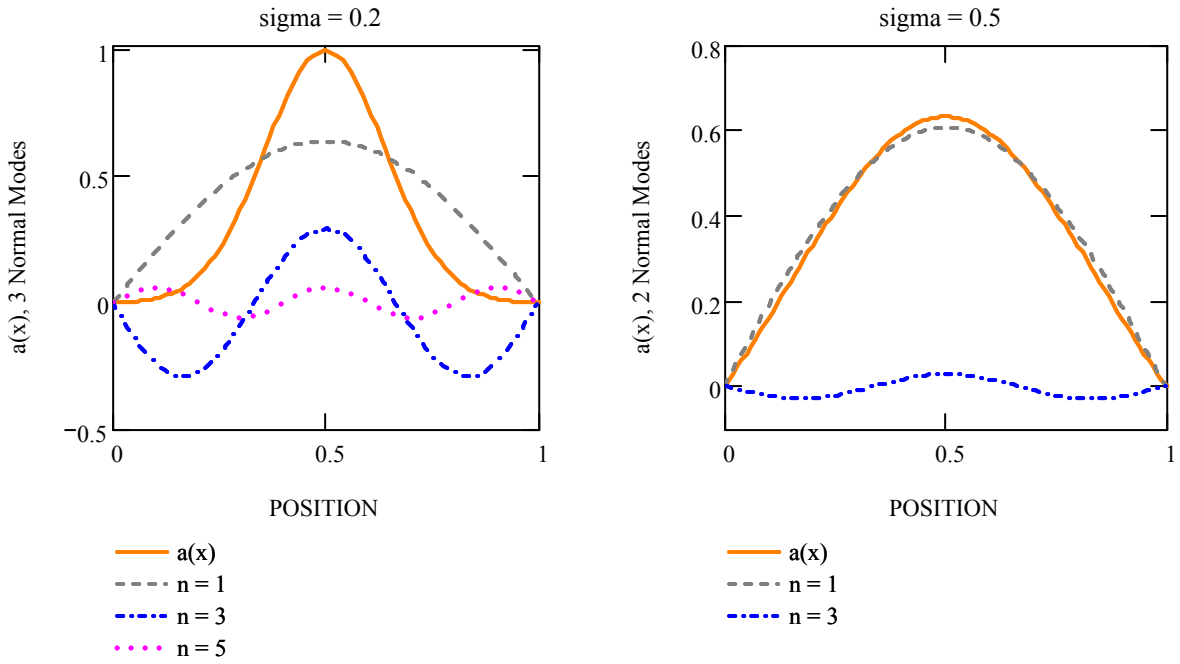
where we have defined $a(x)_M = q(x,0)_M$. That $M \approx 29$ does a good job for $\sigma = 0.05$ is illustrated in the following figure, which plots $a_x(x)_M$ for several values of M. Notice that as M increases $a_x(x)_M$ more faithfully represents the function $a(x)$.



The next 2 figures show the same sort of thing for $\sigma = 0.2$ and $\sigma = 0.5$, but in a more direct fashion. This figures on the left plots the difference $a(x) - a(x)_5$ for $\sigma = 0.2$, while the figure on the right plots $a(x) - a(x)_3$ for $a_0 = 0.5$. In both cases, the error is < 0.06 for all values of x. Given the overall size of $a(x)$, these also seems like reasonable approximations.



The following two graphs are also somewhat illuminating. They plot the initial condition $a(x)$ along with the individual terms on the rhs of Eq. (27), $\sin\left(\frac{n\pi}{L}x\right)\mathrm{Re}(a_n)$, for $n = 1,\ldots,M$. From the graph for $\sigma = 0.5$ it is not hard to imagine that only the $n = 1$ and $n = 3$ are needed to accurately describe $a(x)$.



OK, so what about the time dependence? Now that we know how many normal modes we need, we can simply use Eq. (26) [where $\mathrm{Re}(a_n)$ is calculated with Eq. (24)] with the appropriate value of M. On the class web site there are videos of the resulting wave motion for all three values of σ discussed here. Both the $\sigma = 0.2$ and $\sigma = 0.5$ videos also show the motion of the individual normal modes that are used to produce the approximation $q(x,t)_M$.

Exercises

*__10.1__ Show that $\mathrm{Re}(a_n)\cos(\omega_n t) - \mathrm{Im}(a_n)\sin(\omega_n t)$ can be expressed more succinctly as $\mathrm{Re}\left(a_n e^{i\omega_n t}\right)$. Thus Eq. (6) can be alternatively expressed as $q_{(n)}(x,t) = \sin(k_n x)\mathrm{Re}\left(a_n e^{i\omega_n t}\right)$.

*__10.2__ In the notes it is stated that $\int_0^L \sin\left(\frac{m\pi}{L}x\right)\sin\left(\frac{n\pi}{L}x\right)dx$ is nonzero only if $m = n$ (where m and n are both integers). Using the trig identities for $\cos(x+y)$ and $\cos(x-y)$, do this integral and show that this statement is indeed true.

*__10.3 An initial value problem__. Here we solve an initial value problem with the initial conditions

$$a(x) = 3\sin\left(\frac{2\pi x}{L}\right), \qquad b(x) = 0$$

(**a**) Graph $a(x)$. Does it satisfy Eq. (3), the boundary conditions?
(**b**) Find analytic solutions for $\mathrm{Re}(a_n)$ and $\mathrm{Im}(a_n)$ for this problem.
(**c**) Thus write down the solution $q(x,t)$ for this problem. What is special about this solution?

**__10.4 Another initial value problem__. Here we solve an initial value problem with the initial conditions

$$a(x) = \begin{cases} \dfrac{4h}{L}x & 0 \le x < L/4 \\ \dfrac{4h}{3L}(L-x) & L/4 \le x \le L \end{cases}, \qquad b(x) = 0$$

(**a**) Carefully graph $a(x)$ (either by hand or using a computer program). Does it satisfy Eq. (3), the boundary conditions?
(**b**) Show that $\mathrm{Im}(a_n) = 0$ and $\mathrm{Re}(a_n) = \dfrac{32}{3}h\dfrac{\sin(n\pi/4)}{n^2\pi^2}$ (Either do the integrals by hand, consult an integral table, or use a program like Mathcad, and then simplify.)
(**c**) Thus write down the solution $q(x,t)$ for this initial-value problem.

Introduction to Fourier Series

Overview and Motivation: Fourier series is based on the idea that many functions of interest can be represented as a linear combination of harmonic functions. Is this cool, or what?

Key Mathematics: Fourier Series! And some facts about integrals of odd and even functions.

I. An Observation

We have already been treading in Fourier-series territory. You should recall in the last lecture that we wrote the general solution $q(x,t)$ to the wave equation as a linear combination of normal-mode solutions. Well, these normal mode solutions are harmonic (in both space and time). To write another function as a linear combination of harmonic functions is the basic idea of Fourier series.

As a fairly simple example from last time, let's consider Eq. (8) from those lecture notes, which can be written as

$$a(x) = \sum_{n=1}^{\infty} \mathrm{Re}(a_n) \sin\left(\tfrac{n\pi}{L} x\right). \tag{1}$$

This is a profound equation. It says that we can write the function $a(x)$, which is fairly arbitrary, as a linear combination of the harmonic functions $\sin\left(\tfrac{n\pi}{L} x\right)$. The price we must pay is that we need an infinite number of these functions to describe $a(x)$. However, as we discussed in the last lecture notes, we often need only a few of these functions to accurately describe the function $a(x)$.

You should also recall that last time we found an equation for the coefficient $\mathrm{Re}(a_n)$ of each harmonic function. Without such an equation Eq. (1) might be theoretically interesting, but it would not be of much use. That equation is

$$\mathrm{Re}(a_n) = \frac{2}{L} \int_0^L \sin\left(\tfrac{n\pi}{L} x\right) a(x)\, dx. \tag{2}$$

As we shall see below, equations such as Eqs. (1) and (2) are the essence of Fourier Series theory.

Our formal discussion of Fourier series will be limited to one independent variable, which we call x. The variable x does not necessarily represent a spatial position, however. There are many cases when one is interested in using Fourier series to represent what is happening in time.

II. Fourier Series Equations

The theory of Fourier series starts by considering a function, which we will call $f(x)$, on the symmetric interval $-L \le x \le L$. If $f(x)$ is a "good" function[1] then we can represent $f(x)$ as a linear combination of harmonic functions,

$$f(x) = \alpha_0 + \sum_{n=1}^{\infty} \left[\alpha_n \cos\left(\tfrac{n\pi}{L} x\right) + \beta_n \sin\left(\tfrac{n\pi}{L} x\right) \right]. \tag{3}$$

The amplitudes α_n and β_n are known as the Fourier coefficients of the function $f(x)$. There are a several things to point out here. The first is that the harmonic functions in the series have a period (or wavelength) of $2L/n$. Thus each harmonic function has the periodicity $2L$ of the interval. In fact, the sum in Eq. (3) includes all linearly independent harmonic functions with periodicity $2L$. Second, the average value of an harmonic function over an interval of periodicity is zero. Thus, the coefficient α_0 is needed to represent functions whose average value is not zero. Indeed, as we shall see, α_0 is the average value of the function $f(x)$.

As mentioned above, the representation of a function by a linear combination of harmonic functions isn't that useful unless we know how to calculate the coefficients α_0, α_n, and β_n. Fortunately, expressions for the coefficients are fairly simple and are given by

$$\alpha_0 = \frac{1}{2L} \int_{-L}^{L} f(x)\, dx, \tag{4a}$$

$$\alpha_n = \frac{1}{L} \int_{-L}^{L} f(x) \cos\left(\tfrac{n\pi}{L} x\right) dx, \tag{4b}$$

$$\beta_n = \frac{1}{L} \int_{-L}^{L} f(x) \sin\left(\tfrac{n\pi}{L} x\right) dx. \tag{4c}$$

[1] In typical physicist fashion we will dodge the question of what exactly makes a function "good". If you are interested, there are plenty of text books that discuss this point, including Dr. Torre's text *FWP*.

Now you may be wondering where these equations came from, but you have seen the derivation of formulae equivalent to Eq. (4) several times before. The last time was in the last lecture notes when we obtained Eq. (2) from Eq. (1). *The key is to multiply Eq. (3) by one of the harmonic functions and integrate over the proper interval.*

As an example, let's derive Eq. (4b). Starting with Eq. (3), we multiply it by $\cos\left(\frac{m\pi x}{L}\right)$ (notice the m) and integrate from $-L$ to L, which gives us

$$\int_{-L}^{L} f(x)\cos\left(\tfrac{m\pi}{L}x\right)dx = \alpha_0 \int_{-L}^{L} \cos\left(\tfrac{m\pi}{L}x\right)dx + \sum_{n=1}^{\infty}\left[\alpha_n \int_{-L}^{L} \cos\left(\tfrac{n\pi}{L}x\right)\cos\left(\tfrac{m\pi}{L}x\right)dx + \beta_n \int_{-L}^{L} \sin\left(\tfrac{n\pi}{L}x\right)\cos\left(\tfrac{m\pi}{L}x\right)dx\right] \tag{5}$$

For $m \geq 1$ there is only one nonzero integral on the rhs of this equation,

$$\int_{-L}^{L} \cos\left(\tfrac{m\pi}{L}x\right)\cos\left(\tfrac{m\pi}{L}x\right)dx = L\,. \tag{6}$$

Equation (5) thus greatly simplifies to

$$\int_{-L}^{L} f(x)\cos\left(\tfrac{m\pi}{L}x\right)dx = \alpha_m L\,, \tag{7}$$

which can be solved for α_m, resulting in Eq. (4b) (after replacing m by n).

III. Some Examples

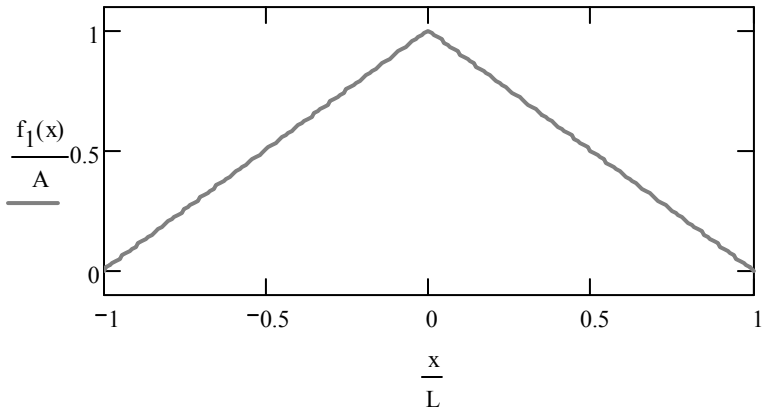
A. Triangle Function

Let's first look at the function,

$$f_1(x) = \begin{cases} \frac{A}{L}x + A & -L \leq x < 0 \\ -\frac{A}{L}x + A & 0 \leq x \leq L \end{cases}, \tag{8}$$

which is plotted in the figure on the top of the next page.

To use the Fourier-series representation of this function we must first calculate the Fourier coefficients using Eq. (4). Before we go ahead and try to calculate the integrals, let's notice a few things that will make the calculations simpler. First, Eq.



(4a) tells us that α_0 is simply the average of the function $f(x)$ on the interval $-L$ to L. From the graph we see that this is $A/2$, so without doing any math we have

$$\alpha_0 = \frac{A}{2}. \tag{9}$$

Second, notice that $f(x)$ is an even function. [An even function has the property $f_{even}(-x) = f_{even}(x)$.] Now Eq. (4c) is the integral of the product of this even function with the odd function $\sin\left(\frac{n\pi}{L}x\right)$. [An odd function is defined via $f_{odd}(-x) = -f_{odd}(x)$.] Now the product of an odd function and an even function is an odd function, and the integral of an odd function over a symmetric interval about zero (such as $-L$ to L) is zero. Thus, again without explicitly calculating the integral in Eq. (4c) we have for this example

$$\beta_n = 0 \tag{10}$$

We are left with determining the coefficients α_n. Even here things are simpler than at first glance: we can use a simplifying fact about integrals of even functions over a symmetric interval about $x = 0$. The simplification is that the integral of an even function over a symmetric interval is equal to twice the integral of the function over the positive (or negative) portion of the interval. Now $\cos\left(\frac{m\pi}{L}x\right)$ is an even function, and the product of two even functions is an even function. With the simplifying fact and Eqs. (4b) and (8) we have

$$\alpha_n = \frac{2}{L}\int_0^L \left(-\tfrac{A}{L}x + A\right)\cos\left(\tfrac{n\pi}{L}x\right)dx. \tag{11}$$

Using Mathcad, for example, the integral is easily evaluated, resulting in

$$\alpha_n = \frac{2A}{n^2\pi^2}\left[1-\cos(n\pi)\right]. \tag{12}$$

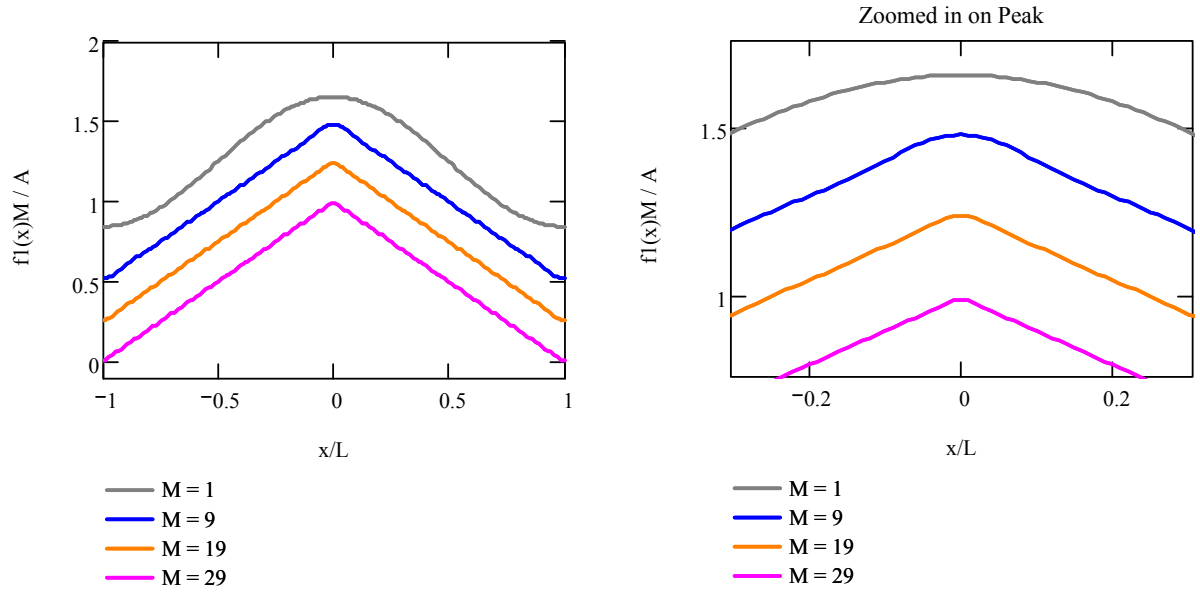
Using Eqs. (9), (10), and (12) in Eq. (3) produces the Fourier representation of $f_1(x)$,

$$f_1(x) = \frac{A}{2} + 2A\sum_{n=1}^{\infty}\left[\frac{1-\cos(n\pi)}{n^2\pi^2}\cos\left(\frac{n\pi}{L}x\right)\right]. \tag{13}$$

As discussed in the last lecture, in practice we use a truncated version of an infinite-series representation such as that in Eq. (13). Following that lecture, we write the truncated version of Eq. (13) as

$$f_1(x)_M = \frac{A}{2} + 2A\sum_{n=1}^{M}\left[\frac{1-\cos(n\pi)}{n^2\pi^2}\cos\left(\frac{n\pi}{L}x\right)\right]. \tag{14}$$

So where should we cut off the series? To get some idea, let's graphically look at Eq. (14) for several values of M. As shown in the following figure, the series with $M = 9$, 19, and 29 all do a reasonable job of representing the original function, with the major difference being the sharpness of the peak at $x = 0$, which is clearly visible in the rhs graph.[2] That the function near this point is hard to represent with an harmonic series isn't surprising. Because $f_1(x)$ has a kink at $x = 0$, its first derivative is undefined there.



[2] Although hard to see in the lhs graph, there is also some rounding of the function at the ends of the interval.

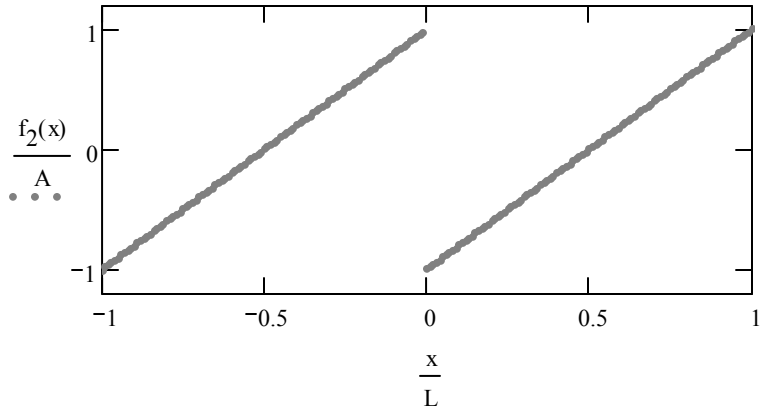
Conversely, the harmonic functions that make up the Fourier series are differentiable at that point; thus for any finite value of M, $f_1(x)_M$ is also be differentiable at $x = 0$.

B. Sawtooth Function

Let's finish up this introduction to Fourier series with another example. This time we look at the function

$$f_2(x) = \begin{cases} \frac{2A}{L}x + A & -L \le x < 0 \\ \frac{2A}{L}x - A & 0 \le x \le L \end{cases}, \tag{15}$$

which is plotted in the next figure. Notice that the function is discontinuous at $x = 0$. Because the harmonic functions are all continuous, you might expect some difficulty in representing this function with a Fourier series. Indeed, there is a major problem, as we shall shortly see.



Again we use Eq. (4) to calculate the Fourier coefficients. As before, the function $f_2(x)$ has enough symmetry to make some of the calculations trivial. We first note from the graph that the average value of $f_2(x)$ is zero, so $\alpha_0 = 0$. Notice also that $f_2(x)$ is odd, which means $f_2(x)\cos\left(\frac{n\pi}{L}x\right)$ is odd, and so this time $\alpha_n = 0$. Similarly, $f_2(x)\sin\left(\frac{n\pi}{L}x\right)$ is even, so we can the equation for β_n simplifies to

$$\beta_n = \frac{2}{L}\int_0^L \left(\frac{2A}{L}x - A\right)\sin\left(\frac{n\pi}{L}x\right)dx. \tag{16}$$

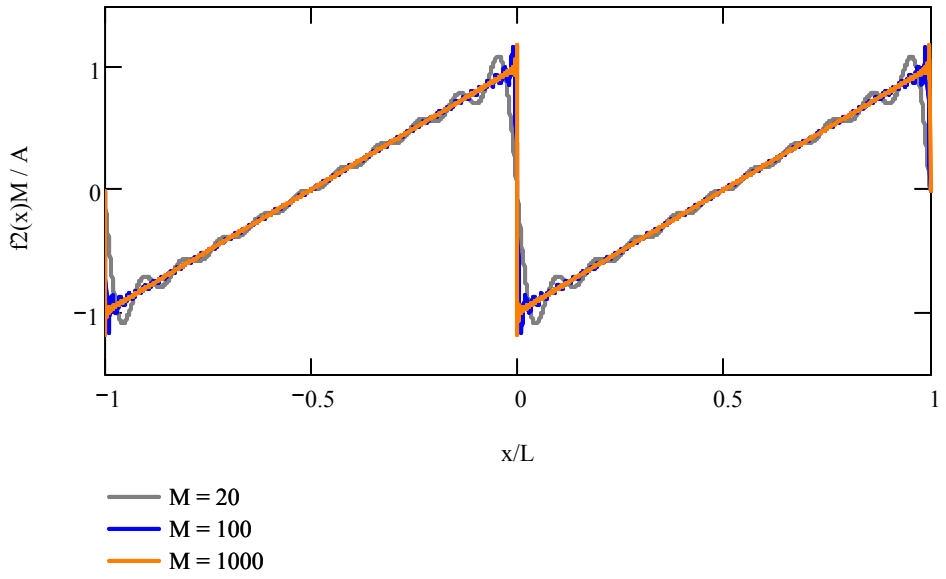
Again, Mathcad can do the integral, and it gives us

$$\beta_n = -\frac{2A}{n\pi}\left[1+\cos(n\pi)\right], \tag{17}$$

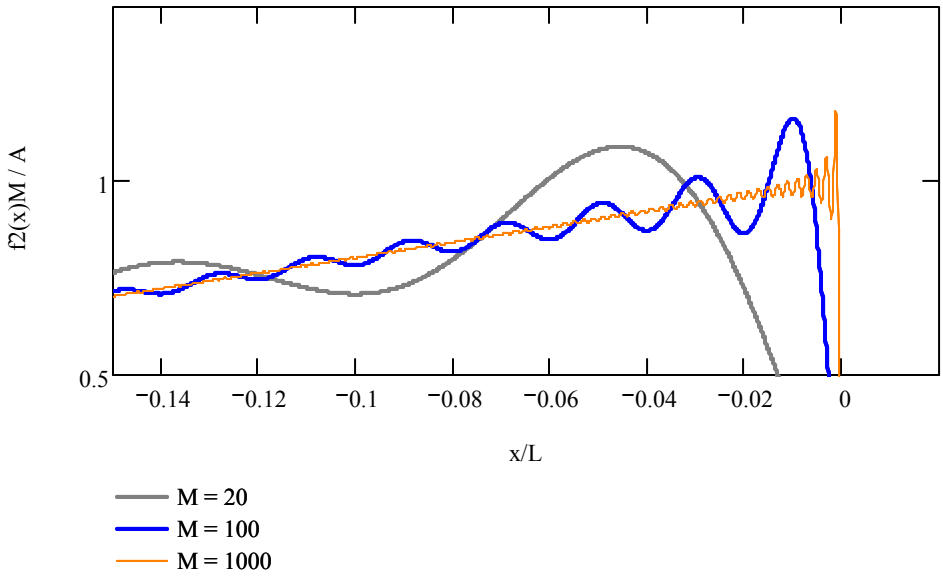
So the truncated Fourier representation of the function $f_2(x)$ can be written as

$$f_2(x)_M = -2A\sum_{n=1}^{M}\left[\frac{1+\cos(n\pi)}{n\pi}\sin\left(\tfrac{n\pi}{L}x\right)\right]. \tag{18}$$

This function is plotted in the next figure for several values of M. Notice that using even a large number of terms does not do justice to the original function. The problem is due to the discontinuity, as was alluded to above.



In fact, something quite pathological happens near the discontinuity, as illustrated in the next figure, where we zoom in on a section of the above graph. As the figure clearly illustrates, there is an overshoot of the truncated Fourier series, and the size of the overshoot does not decrease as the number of terms increases. This overshoot, which is known as the **Gibbs phenomenon**, happens whenever we try to represent a discontinuous function with a (truncated) Fourier series. Notice that the Gibbs phenomenon also occurs for this function at the two ends of the interval. This is because $f_2(L) \neq f_2(-L)$, whereas, the harmonic functions in the Fourier series all have the same value at $-L$ and L.



Summarizing, we have seen how to represent a function on a symmetric interval as a linear combination of harmonic functions that have the periodicity of that interval. If the function is continuous, the representation works well. If the function has a discontinuity, then the representation it not without its difficulties.

Exercises

*__11.1__ Obtain Eq. (4a), the expression for α_0, from Eq. (3).

*__11.2 An integral involving harmonic functions__. In deriving Eq. (6) from Eq. (5) we used the fact that $\int_{-L}^{L} \sin\left(\frac{n\pi}{L}x\right)\cos\left(\frac{m\pi}{L}x\right)dx = 0$ for all integers n and m. Using the trig identities for $\sin(x+y)$ and $\sin(x-y)$, do this integral and show that this equation is indeed true.

*__11.3 Odd and even functions__. Using the basic definitions of even and odd function, $f_{even}(-x) = f_{even}(x)$ and $f_{odd}(-x) = -f_{odd}(x)$, show that the following statements are true.
(**a**) The product of two even functions is even.
(**b**) The product of two odd functions is even.
(**c**) The product of an odd function and an even function is odd.

*__11.4 Integrals of odd and even functions__.

(**a**) If $f(x)$ is an odd function, show that $\int_{-L}^{L} f(x)\,dx = 0$.

(**b**) If $f(x)$ is an even function, show that $\int_{-L}^{L} f(x)\,dx = 2\int_{0}^{L} f(x)\,dx$.

*__11.5__ Starting with Eq. (11) and using integration by parts (where appropriate) derive Eq. 12).

**__11.6 A Fourier series example__. Consider the function

$$f_3(x) = \begin{cases} 0 & -L \le x < -L/2 \\ A & -L/2 \le x \le L/2 \\ 0 & L/2 \le x \le L \end{cases}, \qquad (15)$$

(**a**) Carefully graph this function.
(**b**) Find the Fourier coefficients of this function.
(**c**) Plot $f_3(x)$ and the truncated Fourier expansions of $f_3(x)$ for $M = 1$, 5, and 10.
(**d**) Identify all places where the Gibbs phenomenon occurs.

*__11.7__ Identify whether the following functions are odd, even, or neither. x^3, e^{-x2}, $erf(x)$, $\cosh(x)$, $\sinh(x)$.

Complex Fourier Series

Overview and Motivation: We continue with our discussion of Fourier series, which is all about representing a function as a linear combination of harmonic functions. The new wrinkle is that we now use complex forms of the harmonic functions.

Key Mathematics: More Fourier Series! And a cute trick that often comes in handy when calculating integrals.

I. The Complex Fourier Series

Last time we introduced Fourier Series and discussed writing a function $f(x)$ defined on the interval $-L \le x \le L$ as

$$f(x) = \alpha_0 + \sum_{n=1}^{\infty} \left[\alpha_n \cos\left(\tfrac{n\pi x}{L}\right) + \beta_n \sin\left(\tfrac{n\pi x}{L}\right) \right], \tag{1}$$

where the Fourier coefficients are given as

$$\alpha_0 = \frac{1}{2L} \int_{-L}^{L} f(x)\, dx, \tag{2a}$$

$$\alpha_n = \frac{1}{L} \int_{-L}^{L} f(x) \cos\left(\tfrac{n\pi x}{L}\right) dx, \tag{2b}$$

$$\beta_n = \frac{1}{L} \int_{-L}^{L} f(x) \sin\left(\tfrac{n\pi x}{L}\right) dx. \tag{2c}$$

While there is nothing wrong with this description of Fourier Series, it is often advantageous to use the complex representations of the sine and cosine functions,

$$\cos\left(\tfrac{n\pi x}{L}\right) = \frac{1}{2}\left(e^{in\pi x/L} + e^{-in\pi x/L}\right), \tag{3a}$$

$$\sin\left(\tfrac{n\pi x}{L}\right) = \frac{1}{2i}\left(e^{in\pi x/L} - e^{-in\pi x/L}\right). \tag{3a}$$

If we insert these expressions into Eq. (1) we obtain

$$f(x) = \alpha_0 + \frac{1}{2}\sum_{n=1}^{\infty}\left[\alpha_n\left(e^{in\pi x/L} + e^{-in\pi x/L}\right) - i\beta_n\left(e^{in\pi x/L} - e^{-in\pi x/L}\right)\right], \tag{4}$$

which can be rearranged as

$$f(x) = \alpha_0 + \frac{1}{2}\sum_{n=1}^{\infty}\left[(\alpha_n - i\beta_n)e^{in\pi x/L} + (\alpha_n + i\beta_n)e^{-in\pi x/L}\right]. \tag{5}$$

This doesn't look any simpler, but notice what happens if we define a new set of coefficients (which are simply linear combinations of the of the current coefficients a_n and β_n),

$$c_0 = \alpha_0 \tag{6a}$$

$$c_n = \tfrac{1}{2}(\alpha_n - i\beta_n) \tag{6b}$$

$$c_{-n} = \tfrac{1}{2}(\alpha_n + i\beta_n) \tag{6c}$$

Then we can write Eq. (5) as

$$f(x) = c_0 + \sum_{n=1}^{\infty}\left[c_n e^{in\pi x/L} + c_{-n}e^{-in\pi x/L}\right], \tag{7}$$

or even more simply as

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L}\,. \tag{8}$$

Using Eq. (2) it is not hard to show that the coefficients c_n in Eq. (6) are given by

$$c_n = \frac{1}{2L}\int_{-L}^{L} f(x)\,e^{-in\pi x/L}\,dx\,. \tag{9}$$

Equations (8) and (9) are known as the **complex Fourier series** representation of the function $f(x)$. Notice that with the complex representation there is only one expression needed for all of the Fourier coefficients.

There is another way to obtain Eq. (9), which is to use the same trick that we have used several times before to find coefficients of the harmonic functions: multiply Eq. (8) by the proper function and integrate! Let's say we want to find the mth coefficient c_m. We then multiply Eq. (8) by $e^{-im\pi x/L}$ (notice the minus sign in the exponent!) and integrate on x from $-L$ to L, which produces

$$\int_{-L}^{L} f(x) e^{-im\pi x/L}\, dx = \sum_{n=-\infty}^{\infty} c_n \int_{-L}^{L} e^{i(n-m)\pi x/L}\, dx\,. \tag{10}$$

Now, as before, only one integral on the rhs is nonzero. That is the integral with $n = m$, and its value is $2L$. Eq. (10) thus simplifies to

$$\int_{-L}^{L} f(x) e^{-im\pi x/L}\, dx = c_m 2L\,, \tag{11}$$

which is equivalent to Eq. (9). That is pretty much it for the setup of the complex Fourier series.

II. An Example Revisited

Let's look at an example that we looked at last time, the triangle function

$$f_1(x) = \begin{cases} \frac{A}{L}x + A & -L \le x < 0 \\ -\frac{A}{L}x + A & 0 \le x \le L \end{cases}, \tag{12}$$

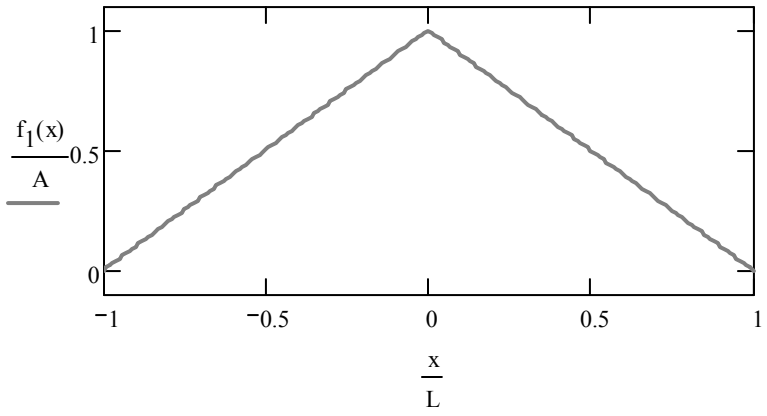
which is plotted on the top of the next page.

Let's use Mathcad to evaluate the c_n's. Inserting Eq. (12) into Eq. (9)

$$c_n = \frac{1}{2L}\left\{ \int_{-L}^{0} \left(\tfrac{A}{L}x + A\right) e^{-in\pi x/L}\, dx + \int_{0}^{L} \left(-\tfrac{A}{L}x + A\right) e^{-in\pi x/L}\, dx \right\} \tag{13}$$

and asking Mathcad to evaluate this expression results in

$$c_n = A\frac{1-\cos(n\pi)}{n^2\pi^2}\,. \tag{14}$$



Not this is OK, as long as we do not use it for more than it is worth: for any nonzero value of n Eq. (14) is perfectly fine. But what about the case of $n=0$? Then this expression is undefined. What this means is that we must explicitly set $n=0$ in Eq. (13) and reevaluate it. But for $n=0$, we see from Eq. (9) that c_0 is just the average value of the function, which is $A/2$. Putting this all together we can represent the function $f_1(x)$ as

$$f_1(x)=\frac{A}{2}+A\sum_{\substack{n=-\infty\\(n\neq 0)}}^{\infty}\frac{1-\cos(n\pi)}{n^2\pi^2}e^{in\pi x/L} \tag{15}$$

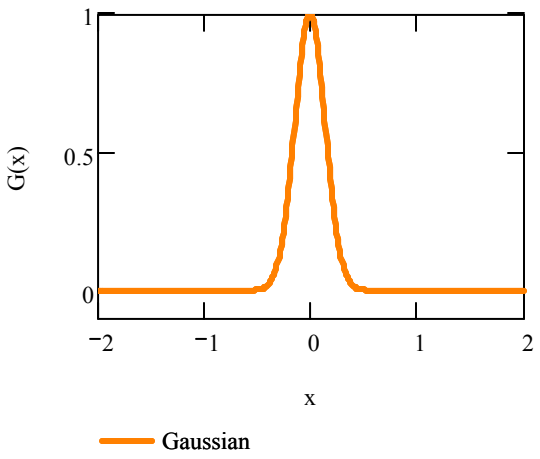
Now this is a valid representation of the function $f_1(x)$, but you may be wondering about something. We know that the function $f_1(x)$ is real, but the rhs of Eq. (15) appears to have an imaginary part, because $e^{in\pi x/L}=\cos\left(\frac{n\pi x}{L}\right)+i\sin\left(\frac{n\pi x}{L}\right)$. So what is the deal? Well, it is not too difficult to see that the imaginary part of each positive-n term is exactly cancelled by the imaginary part of the corresponding negative-n term. So, Eq. (15) is indeed real.

III. The Gaussian Function

Let's take another look at the Gaussian function and think a bit about representing it as a Fourier Series. You should recall that the Gaussian function is defined as

$$G_\sigma(x)=e^{-x^2/\sigma^2}, \tag{16}$$

where σ is known as the width parameter. Let's assume in this example that $L>>\sigma$. Then we have something like the following picture, where we have set $\sigma=0.2$ and $L=2$.



Let's calculate the coefficients c_n. Using Eq. (9) we have

$$c_n = \frac{1}{2L}\int_{-L}^{L} e^{-x^2/\sigma^2}\; e^{-in\pi x/L}\; dx\,. \tag{17}$$

Now this integral can be expressed in terms of the error function, which is the integral of the Gaussian function, but the expression is pretty messy. However, there is an approximate solution to the integral in Eq. (17) that is quite simple and very accurate, as we now show. For the conditions that we assumed, namely $L >> \sigma$, the Gaussian function is nearly zero for $|x| \geq L$. Because of this we can extend the limits of integration in Eq. (17) to $\mp\infty$, and with very little loss of accuracy we can write

$$c_n = \frac{1}{2L}\int_{-\infty}^{\infty} e^{-x^2/\sigma^2}\; e^{-in\pi x/L}\; dx\,, \tag{18}$$

We can also take advantage of the properties of integrals of odd and even functions if we write $e^{-in\pi x/L} = \cos(n\pi x/L) - i\sin(n\pi x/L)$, which turns Eq. (18) into

$$c_n = \frac{1}{2L}\int_{-\infty}^{\infty} e^{-x^2/\sigma^2}\; \left[\cos(n\pi x/L) - i\sin(n\pi x/L)\right] dx\,. \tag{19}$$

Now the Gaussian function is even, so the integral of $e^{-x^2/\sigma^2}\left[-i\sin(n\pi x/L)\right]$ is zero, and so we are left with

$$c_n = \frac{1}{2L}\int_{-\infty}^{\infty} e^{-x^2/\sigma^2}\,\left[\cos(n\pi x/L)\right]dx\,. \tag{19}$$

It so happens that this integral has a nice analytic solution. Using the (fairly well-known) result (which you can find in any table of integrals)

$$\int_{-\infty}^{\infty} e^{-x^2/\sigma^2}\,\cos(\beta x)dx = \sqrt{\pi}\sigma\, e^{-\beta^2\sigma^2/4}, \tag{20}$$

we can identify $n\pi/L$ in Eq. (19) as β in Eq. (20), so we have for the coefficients

$$c_n = \frac{\sqrt{\pi}\sigma}{2L} e^{-n^2/(2L/\pi\sigma)^2}\,. \tag{21}$$

Now this is pretty cool: as a function of n, c_n is also a Gaussian, and its width parameter is $2L/(\pi\sigma)$. Notice that this width parameter is inversely proportional to the width parameter σ of the original Gaussian function $G_\sigma(x) = e^{-x^2/\sigma^2}$.[1]

We can now use Eq. (21) in Eq. (8) and represent a Gaussian function (on the interval $-L \le x \le L$) as

$$G_\sigma(x) = \frac{\sqrt{\pi}\sigma}{2L}\sum_{n=-\infty}^{\infty} e^{-n^2/(2L/\pi\sigma)^2} e^{in\pi x/L}\,. \tag{22}$$

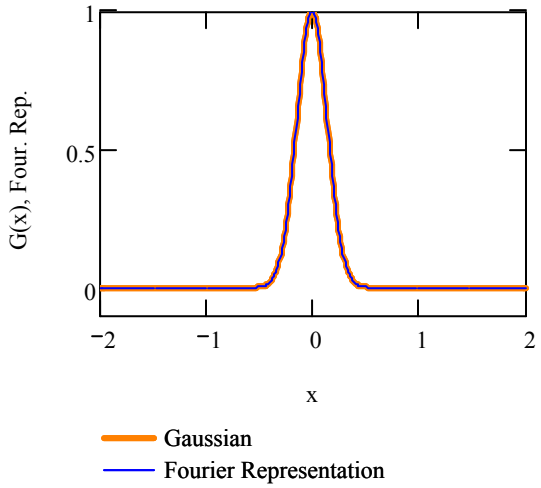
Let's look at the original Gaussian function $G_\sigma(x)$ and its (truncated) Fourier representation,

$$G_\sigma(x)_M = \frac{\sqrt{\pi}\sigma}{2L}\sum_{n=-M}^{M} e^{-n^2/(2L/\pi\sigma)^2} e^{in\pi x/L}\,. \tag{23}$$

So how many terms do we need; that is, how large does M need to be in Eq. (23)? We can get some idea by considering what happens to the coefficients c_n [see Eq. (21)] as $|n|$ gets larger. For a Gaussian function, if the argument is several times larger than the width parameter, then the Gaussian function is very close to zero. Thus, we need to choose M such that it is a few times larger than the width parameter $2L/(\pi\sigma)$. This is illustrated in the next figure, where we have used $M = 20$, which is

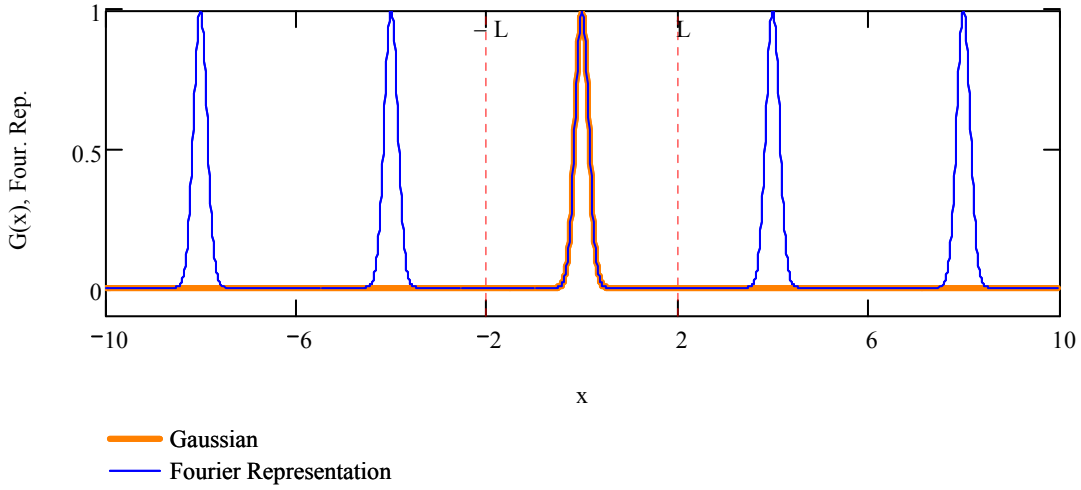
[1] We will see later that this observation is essentially the uncertainty principle of quantum mechanics!

approximately $3\times 2L/(\pi\sigma)$. On the scale of this graph, the truncated Fourier series certainly does a good job of representing the Gaussian function. (As above, we have again set $\sigma = 0.2$ and $L = 2$).



However, there is an inherent limitation to using Fourier series to represent a nonperiodic function such as a Gaussian. That limitation is illustrated in the next figure, which plots the Gaussian and its Fourier series over an interval larger than $-L \le x \le L$. Within the interval the match is very good (as we saw in the last graph), but outside the interval the match is pretty lousy. Why? Well, that is because the harmonic functions that make up the Fourier series all repeat on any interval with length $2L$. Thus, the Fourier representation of the Gaussian function has periodicity $2L$.

Well, you might say that there is no problem here. I'll just pick a value of L that is



larger than any value of x where I might want to evaluate the original function. That might work in practice, but we might also ask the question: is there a Fourier-series representation that will work for all x? The answer is yes, and we will discuss that in a few lectures after this one.

Right now I just want to point out that getting to such a representation is not at all trivial. Consider the following. We have represented the Gaussian as a linear combination of harmonic functions $e^{in\pi x/L}$. If we want to use a Fourier representation for all x, then somehow we must take the limit where $L \to \infty$. What does that mean for the harmonic functions? It looks like all of the harmonic functions will simply become equal to 1 (which seems pretty bad!). There is a resolution to this dilemma, but this illustrates that taking the $L \to \infty$ limit of the Fourier-series representation is somewhat nontrivial.

Exercises

*__12.1__ Calculate the integral on the rhs of Eq. (10) and show that it is nonzero only if $n = m$.

*__12.2__ Consider the result for the coefficient for the triangle function, $c_n = A\dfrac{1-\cos(n\pi)}{n^2\pi^2}$, which is undefined for $n = 0$. Use l'Hôspital's rule to show that as $n \to 0$, $c_n \to A/2$, the result for c_0.

*__12.3__ Using Eq. (2) in Eq. (6b), show that c_n is given by Eq. (9).

**__12.4 Fourier series example__. Consider the function $f(x) = \begin{cases} e^{x} & x \le 0 \\ e^{-x} & x > 0 \end{cases}$.

(a) Plot this function. Explain why this function is even?
(b) Find a *real* analytic expression for the Fourier coefficients c_n for this function. (Hint: You can use the fact that $f(x)$ is even to simplify your determination of the coefficients.)
(c) Let $L = 5$. Plot the function and its truncated Fourier representation for several values of M. What is the minimum reasonable value for M necessary to represent $f(x)$ on this interval?

Vector Spaces / Real Space

Overview and Motivation: We review the properties of a vector space. As we shall see in the next lecture, the mathematics of normal modes and Fourier series is intimately related to the mathematics of a vector space.

Key Mathematics: The concept and properties of a vector space, including addition, scalar multiplication, linear independence and basis, inner product, and orthogonality.

I. Basic Properties of a Vector Space

You are already familiar with several different vector spaces. For example, the set of all real numbers forms a vector space, as does the set of all complex numbers. The set of all position vectors (defined from some origin) is also a vector space. You may not be familiar with the concept of functions as vectors in a vector space. We will talk about that in the next lecture. Here we review the concept of a vector space and discuss the properties of a vector space that make it useful.

A. Vector Addition.

A vector space is a set (of some kind of quantity) that has the operation of **addition** (+) defined on it, whereby two elements **v** and **u** of the set can be added to give another element **w** of the set,[1]

$$\mathbf{w} = \mathbf{u} + \mathbf{v} . \tag{1}$$

There is also an **additive identity** included in the set; this additive identity in known as the zero vector **0**, such that for any vector **v** in the space

$$\mathbf{v} + \mathbf{0} = \mathbf{v} . \tag{2}$$

The addition rule has both **commutative**

$$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u} \tag{3}$$

and **associative**

$$(\mathbf{u} + \mathbf{v}) + \mathbf{w} = \mathbf{u} + (\mathbf{v} + \mathbf{w}) \tag{4}$$

properties.

[1] We denote vector quantities by boldface type and scalars in standard italic type. This is standard practice in most physics journals.

B. Scalar Multiplication

The vector spaces that we are interested in also have another operation defined on them known as **scalar multiplication**, in which a vector $\mathbf{u}$ in the space can be multiplied by either a real or complex number a, producing another vector in the space $\mathbf{v} = a\mathbf{u}$. If we are interested in multiplying the elements of the space by only real numbers it is known as a **real vector space**; if we wish to multiply the elements of the space by complex numbers, then the space is known as a **complex vector space**.

Scalar multiplication must satisfy the following properties for scalars a and b and vectors $\mathbf{u}$ and $\mathbf{v}$,

$$(a+b)\mathbf{u} = a\mathbf{u} + b\mathbf{u}, \tag{5a}$$

$$a(b\mathbf{u}) = (ab)\mathbf{u}, \tag{5b}$$

$$a(\mathbf{u}+\mathbf{v}) = a\mathbf{u} + a\mathbf{v}, \tag{5c}$$

$$1\mathbf{u} = \mathbf{u}, \tag{5d}$$

$$0\mathbf{u} = \mathbf{0}. \tag{5e}$$

None of these properties should be much of a surprise (I hope!)

C. Linear Independence and Basis

The **span** of a subset of m vectors is the set of all vectors that can be written as a linear combination of the m vectors,

$$a_1\mathbf{u}_1 + a_2\mathbf{u}_2 + \ldots + a_m\mathbf{u}_m. \tag{6}$$

The subset of m vectors is **linearly independent** if none of the subset can be written as a linear combination of the other members of the subset. If the subset is **linearly dependent** then we can write at least one of the members as a linear combination of the others, for example

$$\mathbf{u}_m = a_1\mathbf{u}_1 + a_2\mathbf{u}_2 + \ldots + a_{m-1}\mathbf{u}_{m-1}. \tag{7}$$

For a given vector space if there is a maximum number of linearly independent vectors possible, then that number defines the **dimension** N of the vector space.[2] That means if we have identified N linearly independent vectors then those N vectors span the entire vector space. This means that any vector in the space can be written as a linear combination of the set of N independent vectors as

$$\mathbf{v} = v_1 \mathbf{u}_1 + v_2 \mathbf{u}_2 + \ldots + v_N \mathbf{u}_N , \tag{8}$$

or in more compact notation as

$$\mathbf{v} = \sum_{n=1}^{N} v_n \mathbf{u}_n . \tag{9}$$

Furthermore the **coefficients**[3] v_n in Eq. (9) are unique. The vectors $\mathbf{u}_n$ in Eq. (9) are said to form a **basis** for the space. Now Eq. (9) should look strangely familiar. We have some quantity on the lhs that is written as a linear combination of quantities on the rhs. Hum… And you might even ask, assuming that I know the vectors $\mathbf{u}_n$ in Eq. (7), how do I find the coefficients v_n?

D. Inner Product

This last question is most easily answered after we define one more operation on the vector space, known as the **inner product** of two vectors, which we denote $(\mathbf{u},\mathbf{v})$. The inner product returns a scalar, which is a real number for a real vector space or a complex number for a complex vector space. The inner product can be defined in any manner as long as it satisfies the following relationships

$$(\mathbf{u},\mathbf{v}) = (\mathbf{v},\mathbf{u})^* \tag{10a}$$

$$(\mathbf{w}, a\mathbf{v} + b\mathbf{u}) = a(\mathbf{w},\mathbf{v}) + b(\mathbf{w},\mathbf{u}) \tag{10b}$$

Note the complex-conjugate symbol in Eq. (10a). If we are dealing with a real vector space, then we can just ignore the complex-conjugate symbol. Also note that Eq. (10a) implies that the inner product of a vector $\mathbf{u}$ with itself is a real number. It can be shown that Eqs. (10a) and (10b) imply that

[2] If there is not a maximum number of linearly independent vectors, then the space is said to have infinite dimension.

[3] The coefficients v_n are also known as the **scalar components** of $\mathbf{v}$ in the basis $\{\mathbf{u}_1,\ldots,\mathbf{u}_N\}$.

$$(a\mathbf{v}+b\mathbf{u},\mathbf{w})=a^*(\mathbf{v},\mathbf{w})+b^*(\mathbf{u},\mathbf{w}) \tag{10c}$$

$$(a\mathbf{v},b\mathbf{u})=a^*\,b(\mathbf{v},\mathbf{u}) \tag{10d}$$

In physics we are usually interested in vector spaces where

$$(\mathbf{u},\mathbf{u})\geq 0\,,\ (\mathbf{u},\mathbf{u})=0\ \textit{iff}\ \ \mathbf{u}=\mathbf{0}\,. \tag{10e}$$

Such vector spaces are said to have a **positive semi-definite norm** (the norm is defined below).

With these properties of the inner product denoted, we can define the concept of orthogonality. Two nonzero vectors $\mathbf{u}$ and $\mathbf{v}$ are said to be **orthogonal** if their inner product vanishes, i.e., if $(\mathbf{u},\mathbf{v})=0$.

Note that if two vectors are orthogonal, then they are linearly independent. This is easy to see, as follows. Assume the converse, that they are linearly dependent. Then their (assumed) linear dependence means that $\mathbf{u}=a\,\mathbf{v}$, where a is some scalar [see Eq. (7)]. Then the scalar product $(\mathbf{v},\mathbf{u})=(\mathbf{v},a\,\mathbf{v})=a(\mathbf{v},\mathbf{v})$ cannot be zero because $\mathbf{v}$ is not zero [see Eq. (10e)]. Thus they must be linearly independent.

The converse is not true, two linearly independent vectors need not be orthogonal. The proof is given as one of the exercises.

One last thing regarding the inner product. The quantity $\|\mathbf{u}\|=\sqrt{(\mathbf{u},\mathbf{u})}$ is generally known as the **norm** (or size) of the vector $\mathbf{u}$. Often we are interested in vectors whose norm is 1. We can "normalize" any vector $\mathbf{u}$ with scalar multiplication by calculating

$$\hat{\mathbf{u}}=\frac{\mathbf{u}}{\sqrt{(\mathbf{u},\mathbf{u})}}\,. \tag{11}$$

The "hat" over a vector indicates that the vector's norm is 1.

E. Orthogonal Basis

Most of the time that we deal with a basis, the vectors in that basis are orthogonal. That is, their inner products with each other vanish. In this case it is a simple matter to find the components v_n in Eq. (9). Let's say that we want to find the mth component v_m. Then we take the inner product of Eq. (9) with $\mathbf{u}_m$, and we get

$$(\mathbf{u}_m, \mathbf{v}) = \left(\mathbf{u}_m, \sum_{n=1}^{N} v_n \mathbf{u}_n \right) = \sum_{n=1}^{N} v_n (\mathbf{u}_m, \mathbf{u}_n) \tag{12}$$

[This last equality follows from Eq. (10b).] So what happens? Well, there will only be one nonzero inner product on the rhs, $(\mathbf{u}_m, \mathbf{u}_m)$, and so Eq. (12) becomes

$$(\mathbf{u}_m, \mathbf{v}) = v_m (\mathbf{u}_m, \mathbf{u}_m), \tag{13}$$

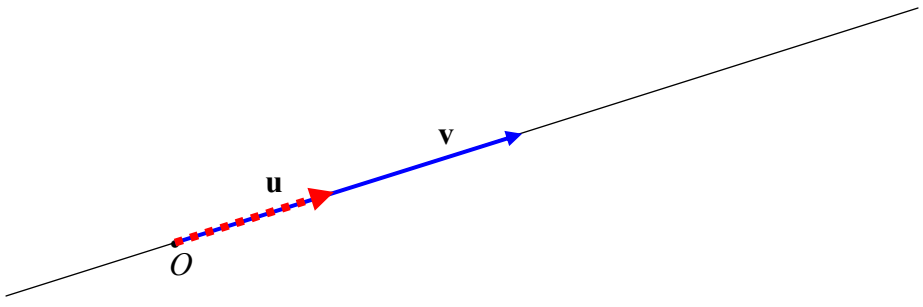
and we can now solve for v_m as

$$v_m = \frac{(\mathbf{u}_m, \mathbf{v})}{(\mathbf{u}_m, \mathbf{u}_m)}. \tag{14}$$

All of this should now look even more strangely familiar. We will get to why that is in the next lecture, but right now we will review a vector space with which you should have some familiarity.

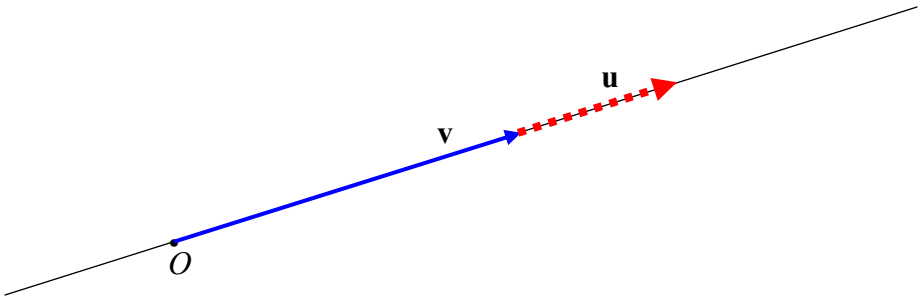
II. 1D Displacement Space

Let's look at a simple example to start. Assume that we have a line drawn somewhere, and on that line we have identified an origin O, as illustrated in the picture below. The vector space that we are interested in consists of all the arrows that start at O and end someplace on the line. The picture also illustrates two of these vectors, one denoted $\mathbf{u}$ and one denoted $\mathbf{v}$.[4]



[4] Note, this vector space is not a vector field. A vector field is the assignment of a vector to each point in space.

So let's talk about some of the math introduced above with respect to this vector space. We first have to define vector addition, which must satisfy Eqs. (1) – (4). Let's go with the standard physics definition of vector addition, whereby we add vectors by the tip-to-tail method, where the one of the arrows is translated (without any rotation) and its tail is placed at the tip of the other arrow, as illustrated in the picture below. Clearly this produces another arrow whose tails is at the origin and head is on the line (and is thus a vector in the space). Eq. (1) is thus satisfied. It should also be clear that we could have translated **v** rather than **u** in this example, and so this definition satisfies Eq. (3), the commutative property of vector addition. We will not illustrate it here, but you should convince yourself that Eq. (4), the associative property is satisfied by the sum of three arrows. What about the zero vector? Well, if Eq. (2) is to be satisfied, it must have no length, and so it must be the arrow that begins and ends at the origin.



What about scalar multiplication? Again, we go with the standard definition, whereby scalar multiplication by a positive number *a* results in an arrow that points in the same direction and is *a* times longer than the original arrow. Multiplication by a negative scalar *b* results in an arrow that points in the opposite direction and is *b* times longer than the original arrow. It should be clear that this definition satisfies all parts of Eq. (5).

What about linear independence and dimension? Pick an arrow, any arrow. Now ask yourself the following question: can I find another arrow that is not a multiple of my first arrow. If the answer is no (which it is), then the vector space has one dimension, and you can use any arrow as the basis for the space. For example, let's say you pick the arrow **u** in the above drawing as your basis. Then the space is one dimensional because you can write any other arrow **v** as

$$\mathbf{v} = a\,\mathbf{u}\,, \tag{15}$$

where a is some scalar. Although we have not yet defined what the inner product is, notice that if we take the inner product of Eq. (15) with $\mathbf{v}$ we get

$$(\mathbf{v},\mathbf{v}) = (a\,\mathbf{u}, a\,\mathbf{u}) = a^2(\mathbf{u},\mathbf{u}), \tag{16}$$

so that

$$a = \pm\frac{\sqrt{(\mathbf{v},\mathbf{v})}}{\sqrt{(\mathbf{u},\mathbf{u})}} = \pm\frac{\|\mathbf{v}\|}{\|\mathbf{u}\|}, \tag{17}$$

with the sign depending upon the sign of a. Now scalar multiplication was defined as multiplying an arrow's length by the multiplying scalar. Thus a is also the + or – ratio of the two vector's lengths. Therefore, for this space the norm must be proportional to the length of the arrow.

So what about the inner product? Also notice the following. Because this is a one dimensional space, this basis $\{\mathbf{u}\}$ is trivially orthogonal, and we can use Eq. (14) (where here a takes the place of v_m) to express the coefficient a in Eq. (15) as

$$a = \frac{(\mathbf{u},\mathbf{v})}{(\mathbf{u},\mathbf{u})}. \tag{18}$$

Together Eqs. (17) and (18) imply

$$(\mathbf{u},\mathbf{v}) = \pm\sqrt{(\mathbf{u},\mathbf{u})}\sqrt{(\mathbf{v},\mathbf{v})} = \pm\|\mathbf{u}\|\,\|\mathbf{v}\|. \tag{19}$$

So which sign do we use? As we now show, it depends upon the relative directions of the two arrows. Let's first consider the case where $\mathbf{u}$ and $\mathbf{v}$ are in the same direction. Then we can write $\mathbf{v} = a\,\mathbf{u}$, where $a > 0$. The we have the following

$$(\mathbf{u},\mathbf{v}) = (\mathbf{u}, a\,\mathbf{u}) = a(\mathbf{u},\mathbf{u}) \tag{20}$$

Because $(\mathbf{u},\mathbf{u})>0$, $(\mathbf{u},\mathbf{v})>0$, and we must use the positive sign if $\mathbf{u}$ and $\mathbf{v}$ are in the same direction. Similarly, if $\mathbf{u}$ and $\mathbf{v}$ are in opposite directions then $a < 0$, and we must use the negative sign.

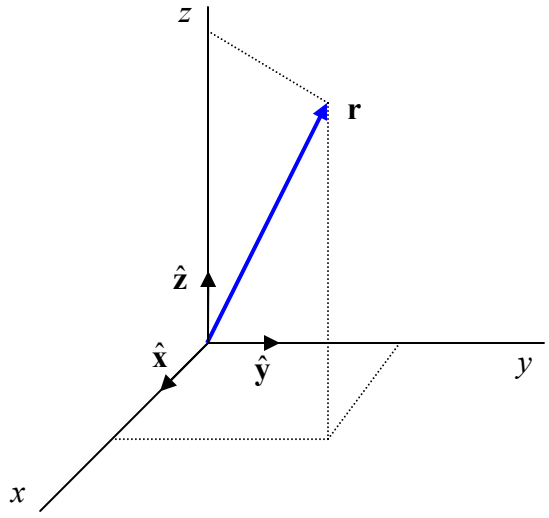
One last comment: notice that nothing we have done here makes us chose the norm to be exactly equal the length of the arrows; it must only be proportional to the length of the arrows. For this space, however, the standard definition of the vector norm is simply the arrow length.

III. Real Space (R^3)

What is real space? It is the extension of this 1D displacement space that we have been discussing to 3 dimensions. That is, it is simply the set of all displacement vectors **r** defined with respect to some fixed origin.

Our discussion here will center on the more practical, at least from a physics point of view. The picture below illustrates the following discussion. In dealing with this space, we typically define a set of three mutually perpendicular axes that pass through the origin, which we label x, y, and z. We also denote three special vectors in this space, the three **unit-norm** vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$, which are three arrows that point along the three axes, respectively. The relative orientations of these three unit vectors are defined by the right-hand-rule (i.e., cross product) through the equation $\hat{\mathbf{z}} = \hat{\mathbf{x}} \times \hat{\mathbf{y}}$. You should convince yourself that these three vectors are linearly independent (given our definitions of vector addition and scalar multiplication discussed in the last section). It is also true that these three vectors are a basis for our vector space, so this vector space is three dimensional. Thus we can write any vector in the space as a linear combination of these three vectors as

$$\mathbf{r} = r_x \hat{\mathbf{x}} + r_y \hat{\mathbf{y}} + r_z \hat{\mathbf{z}} \tag{21}$$



So now we are back to the ever occurring problem of determining the coefficients of some quantity of interest that is expressed as a linear combination of some other quantities. To do this we can again use the inner product, once it is defined. We use the standard definition of the inner product of two vectors in this space

$$(\mathbf{u},\mathbf{v}) = \|\mathbf{u}\|\,\|\mathbf{v}\|\cos(\theta) \tag{22}$$

where θ is the angle between the directions of the two arrows. Notice that this definition reduces to the definition that we came up with for two vectors in our 1D space above, $(\mathbf{u},\mathbf{v}) = \pm\|\mathbf{u}\|\,\|\mathbf{v}\|$, where the sign depends upon the relative directions of the two vectors.

With Eq. (22) it is easy to see that the unit vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ satisfy the following relationships,

$$(\hat{\mathbf{x}},\hat{\mathbf{x}}) = (\hat{\mathbf{y}},\hat{\mathbf{y}}) = (\hat{\mathbf{z}},\hat{\mathbf{z}}) = 1 \tag{23a}$$

$$(\hat{\mathbf{x}},\hat{\mathbf{y}}) = (\hat{\mathbf{y}},\hat{\mathbf{z}}) = (\hat{\mathbf{x}},\hat{\mathbf{z}}) = 0\,. \tag{23b}$$

Eq. (23) defines an **orthonormal basis** for a three dimensional space. That is, the basis is made up of unit vectors [Eq. (23a)] that are all mutually orthogonal [Eq. (23b)].

Using Eq. (23) we can now express the coefficients in Eq. (21) as

$$r_x = \frac{(\hat{\mathbf{x}},\mathbf{r})}{(\hat{\mathbf{x}},\hat{\mathbf{x}})} = (\hat{\mathbf{x}},\mathbf{r}),\quad r_y = \frac{(\hat{\mathbf{y}},\mathbf{r})}{(\hat{\mathbf{y}},\hat{\mathbf{y}})} = (\hat{\mathbf{y}},\mathbf{r}),\quad r_x = \frac{(\hat{\mathbf{z}},\mathbf{r})}{(\hat{\mathbf{z}},\hat{\mathbf{z}})} = (\hat{\mathbf{z}},\mathbf{r}). \tag{24a) – (24c}$$

which enables us to rewrite Eq. (21) as

$$\mathbf{r} = (\hat{\mathbf{x}},\mathbf{r})\hat{\mathbf{x}} + (\hat{\mathbf{y}},\mathbf{r})\hat{\mathbf{y}} + (\hat{\mathbf{z}},\mathbf{r})\hat{\mathbf{z}}\,. \tag{25}$$

Note that Eq. (24) is the specific form of Eq. (14) for the case at hand. Notice also that because the basis vectors have unit norms, the coefficients have an especially simple form: each coefficient is simply the inner product of the respective basis vector with the particular vector of interest.

Lastly, we remark that the inner product between two vectors **r** and **s** can be simply written in terms of the components of those vectors in an orthonormal basis. Let's assume that **r** is given by Eq. (21) and **s** by an analogous equation. Then we can write

$$(\mathbf{r},\mathbf{s}) = \left(r_x\hat{\mathbf{x}} + r_y\hat{\mathbf{y}} + r_z\hat{\mathbf{z}}, s_x\hat{\mathbf{x}} + s_y\hat{\mathbf{y}} + s_z\hat{\mathbf{z}}\right). \tag{26}$$

Now it can be shown that the definition of the inner product [Eq. (22)] satisfies Eq. (10) and so Eq. (26) simplifies to

$$(\mathbf{r},\mathbf{s}) = r_x s_x + r_y s_y + r_z s_z . \tag{27}$$

That is, the inner product of two vectors can be simply expressed as the sum of the products of corresponding components of the two vectors.

Lastly, we remark that when working with vectors in real space we often use a more notationally compact form than that in Eq. (20): we often simply express the vector $\mathbf{r}$ as its triplet of components

$$\mathbf{r} = (r_x, r_y, r_z), \tag{28}$$

leaving the basis vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ as implied. But, when using this notation one must keep in mind that lurking in the background is an implied set of basis vectors.

Exercises

*__13.1 The inner product__
(**a**) Show that Eq. (10a) implies that the inner product of a vector $\mathbf{u}$ with itself is a real number.
(**b**) Using Eqs. (10a) and (10b) show that Eq. (10c) follows.
(**c**) Using Eqs. (10a) and (10b) show that Eq. (10d) follows

*__13.2 Projection__. The projection of a vector $\mathbf{v}$ onto the direction of another vector $\mathbf{u}$ is defined as $\mathbf{p}(\mathbf{v},\mathbf{u}) = \dfrac{(\mathbf{u},\mathbf{v})}{(\mathbf{u},\mathbf{u})}\mathbf{u}$. Consider an orthogonal (but not necessarily normal) basis $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$. Using this basis any vector $\mathbf{v}$ can be written as $\mathbf{v} = v_1\mathbf{u}_1 + v_2\mathbf{u}_2 + v_3\mathbf{u}_3$. Determine expressions for v_1, v_2, and v_3 and thus show that $\mathbf{v}$ can be written as $\mathbf{v} = \mathbf{p}(\mathbf{v},\mathbf{u}_1) + \mathbf{p}(\mathbf{v},\mathbf{u}_2) + \mathbf{p}(\mathbf{v},\mathbf{u}_3)$. That is, the vector $\mathbf{v}$ is simply the sum of its projections onto the orthogonal basis set. In physics we often call these projections the *vector* components of $\mathbf{v}$ in the $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$ basis.

*__13.3__ Consider two linearly independent vectors $\mathbf{u}$ and $\mathbf{v}$ and the vector $\mathbf{w} = \mathbf{v} - \frac{(\mathbf{u},\mathbf{v})}{(\mathbf{u},\mathbf{u})}\mathbf{u}$ made from these two vectors. Assume that the vector space is complex. In this problem you are going to do two separate calculations, both of which show that $\mathbf{w}$ is orthogonal to $\mathbf{u}$. You may find Eqs. (10a) – (10d) useful here.
(**a**) Easy way: Calculate the inner product $(\mathbf{u},\mathbf{w})$ to show that $\mathbf{w}$ is orthogonal to $\mathbf{u}$.
(**b**) Slightly harder way: Calculate the inner product $(\mathbf{w},\mathbf{u})$ to show that $\mathbf{w}$ is orthogonal to $\mathbf{u}$.
(This important result can be used to create an orthogonal basis out of any basis.)

*__13.4__ Show that two linearly independent vectors need not be orthogonal. (Hint: you may find the result of Exercise 13.3 to be helpful here.)

*__13.5__ Assuming that Eq. (10) applies, show that Eq. (27) follows from Eq. (26).

*__13.6__ Use Eq. (27) to find the norm of the vector $\mathbf{r} = r_x\,\hat{\mathbf{x}} + r_y\,\hat{\mathbf{y}} + r_z\,\hat{\mathbf{z}}$. Does your result look familiar?

__13.7__ **__Real space__. A vector $\mathbf{r}$ in real space has components $(4,-1,10)$ in one orthonormal basis. In this same basis a set of vectors is given by $\hat{\mathbf{u}}_1 = \left(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},0\right)$, $\hat{\mathbf{u}}_2 = \left(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},0\right)$, $\hat{\mathbf{u}}_3 = (0,0,-1)$.
(**a**) Show that this set of vectors is orthonormal (and is thus another orthonormal basis).
(**b**) Find the components of $\mathbf{r}$ in this new basis.
(**c**) From the components given in the statement of the problem, find $\|\mathbf{r}\|$.
(**d**) From the components determined in part (**b**), find $\|\mathbf{r}\|$. Is $\|\mathbf{r}\|$ the same as calculated in part (**c**)?

Linear Operators / Functions as Vectors

Overview and Motivation: We first introduce the concept of linear operators on a vector space. We then look at some more vector-space examples, including a space where the vectors are functions.

Key Mathematics: More vector-space math!

I. Linear Operators

A. Definition and Examples

The essential nature of a **linear operator** is contained in its name. The operator part of the name means that a linear operator A operates on any vector $\mathbf{u}$ (in the space of interest) and produces another vector $\mathbf{v}$ in the space. That is, if $\mathbf{u}$ is a vector, then

$$\mathbf{v} = A\mathbf{u} \tag{1}$$

is also vector. The linear part of linear operator means that

$$A(a\,\mathbf{u} + b\,\mathbf{v}) = a\,A\mathbf{u} + b\,A\mathbf{v} \tag{2}$$

is satisfied for all scalars a and b and all vectors $\mathbf{u}$ and $\mathbf{v}$ in the space.

Linear operators come in many different forms. The ones of interest for any given vector space depend upon the problem being solved. When dealing with a vector space of finite dimension, we can always use standard linear-algebra notation to represent the vectors as **column matrices** of length N and the linear operators as **square matrices** of size $N \times N$. For $N = 3$, for example, Eq. (1) can be written as

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}, \tag{3}$$

where v_i, u_i, and A_{ij} are the (scalar) components of $\mathbf{v}$, $\mathbf{u}$, and A, respectively, in some particular orthonormal basis. [1]

As we shall see below, sometimes we are interested in a vector space where the vectors are functions. In that case the linear operators of interest may be linear

[1] For example, if dealing with vectors in real space, the elements in a column vector are often the scalar components (also known as Cartesian coordinates) of that vector in the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$ basis.

differential operators. An example of a **linear differential operator** on a vector space of functions of x is d/dx. In this case Eq. (1) looks like

$$g(x) = \frac{d}{dx} f(x), \tag{4}$$

where $f(x)$ and $g(x)$ are vectors in the space and d/dx is the linear operator.

B. Eigenvalue Problems

An important vector-space problem is the eigenvalue problem. We already have some experience with this problem as part of the process of finding the normal modes of the coupled oscillators. Simply stated, the **eigenvalue problem** is this: for a given linear operator A, what are the vectors $\mathbf{u}$ and scalars λ such that

$$A\mathbf{u} = \lambda\mathbf{u} \tag{5}$$

is satisfied? These vectors $\mathbf{u}$ and scalars λ are obviously special to the operator: when operated on by A, these vectors only change by the scale factor λ. These special vectors $\mathbf{u}$ are known as **eigenvectors** and the values of λ are known as **eigenvalues**. Each eigenvector $\mathbf{u}$ has associated with it a particular eigenvalue λ.

For a vector space of N dimensions (where we are using standard linear algebra notation) the eigenvalues are solutions of the **characteristic equation**

$$\det(A - \lambda I) = 0, \tag{8}$$

where I is the **identity matrix**. As we did when solving the $N = 2$ and $N = 3$ (homework) coupled oscillator problems, substituting the eigenvalues (one at a time!) back into Eq. (5) allows us to find the eigenvectors $\mathbf{u}$.

If the (finite dimension) vector space is complex then Eq. (8) always has solutions.[2] Now here is the cool thing. If the operator is **self-adjoint** (also know as **Hermitian**), which means that its matrix elements satisfy $A_{ji} = A_{ij}^*$, then

(*i*) its eigenvalues are real,
(*ii*) its eigenvectors span the space, and
(*iii*) the eigenvectors with distinct eigenvalues are orthogonal.

Thus, if the operator A is self-adjoint and all eigenvalues are distinct, then those eigenvectors form an orthogonal basis for the space. If the eigenvalues are not

[2] This result is known as the fundamental theorem of algebra.

distinct, an orthogonal basis can still be formed from the eigenvectors. (it just takes a little bit of work.)

Often, however, the eigenvalue problem of interest is on a real vector space. In this case, if A is **symmetric** (that is, the matrix elements of A satisfy $A_{ij} = A_{ji}$), then Eq. (8) will have N real solutions and, again, the associated eigenvectors **u** can be used to form a basis for the vector space.

A famous eigenvalue problem from quantum mechanics is none other than the time-independent **Schrödinger equation**

$$H\psi = E\psi\,, \tag{6}$$

which is an eigenvalue problem on a vector space of functions. Here the vectors are the functions $\psi(x,y,z)$; the operator is the differential operator

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x,y,z); \tag{7}$$

and the eigenvalues are specific values of E.[3] This is perhaps the most important equation in quantum mechanics because the (normalized) eigenvectors describe the (spatial part of the) states of the system with a definite value of energy, and the eigenvalues E are the energies of those states.

II. The Coupled Oscillator Problem Redux

Let's revisit the coupled oscillator problem to see how that problem fits into our discussion of vector spaces. We first review the associated eigenvalue problem that we solved when finding the normal modes, and then we make some remarks about the initial-value problem.

A. The Eigenvalue Problem

Recall, in that problem we started with N equations of motion (one for each object)

$$\ddot{q}_j - \tilde{\omega}^2\left(q_{j-1} - 2q_j + q_{j+1}\right) = 0\,, \tag{9}$$

($j = 1,\ldots,N$), where $q_j(t)$ is the time-dependent displacement of the jth oscillator. We then looked for normal-mode solutions

[3] The function $V(x,y,z)$ is the classical potential energy a particle of mass m.

$$q_j(t) = q_{0,j} e^{i\Omega t}, \tag{10}$$

where all N objects oscillate at the same frequency Ω. By assuming that the solutions had the form of Eq. (10), the N coupled ordinary differential equations became the N coupled algebraic equations

$$\Omega^2 q_{0,j} + \tilde{\omega}^2 \left(q_{0,j-1} - 2q_{0,j} + q_{0,j+1} \right) = 0, \tag{11}$$

which we rewrote as

$$\begin{pmatrix} 2\tilde{\omega}^2 & -\tilde{\omega}^2 & 0 & 0 & \\ -\tilde{\omega}^2 & 2\tilde{\omega}^2 & -\tilde{\omega}^2 & 0 & \\ 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2 & -\tilde{\omega}^2 & \cdots \\ 0 & 0 & -\tilde{\omega}^2 & 2\tilde{\omega}^2 & \\ & & \vdots & & \end{pmatrix} \begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ \vdots \\ q_{0,N} \end{pmatrix} = \Omega^2 \begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ \vdots \\ q_{0,N} \end{pmatrix} \tag{12}$$

Notice that this is exactly of the form of Eq. (5) (the eigenvalue problem) where the vectors are $N-$row column matrices, the linear operator A is an $N \times N$ matrix, and the eigenvalues λ are the squared frequencies Ω^2.

As we previously discovered in solving that problem there are N eigenvectors,

$$\begin{pmatrix} q_{0,1} \\ q_{0,2} \\ q_{0,3} \\ \vdots \\ q_{0,N} \end{pmatrix}_n = \begin{pmatrix} \sin\left(\frac{n\pi}{N+1} 1\right) \\ \sin\left(\frac{n\pi}{N+1} 2\right) \\ \sin\left(\frac{n\pi}{N+1} 3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1} N\right) \end{pmatrix} \tag{13}$$

($n = 1, \ldots, N$), and the nth eigenvector has the eigenvalue

$$\Omega_n^2 = 4\tilde{\omega}^2 \sin^2\left(\frac{n\pi}{2(N+1)} \right). \tag{14}$$

Notice that the eigenvalues are real, as they should be for a symmetric operator. Also, because the eigenvalues are distinct, the eigenvectors from an orthogonal basis for the space.

B. The Initial Value Problem

As part of solving the initial-value problem for this system, we ended up with the equation[4]

$$\begin{pmatrix} q_1(0) \\ q_2(0) \\ q_3(0) \\ \vdots \\ q_N(0) \end{pmatrix} = \sum_{n=1}^{N} \mathrm{Re}(a_n) \begin{pmatrix} \sin\left(\frac{n\pi}{N+1}1\right) \\ \sin\left(\frac{n\pi}{N+1}2\right) \\ \sin\left(\frac{n\pi}{N+1}3\right) \\ \vdots \\ \sin\left(\frac{n\pi}{N+1}N\right) \end{pmatrix}, \tag{15}$$

which we needed to solve for the coefficients $\mathrm{Re}(a_n)$. Let's now place the previous solution of Eq. (15) for the coefficients $\mathrm{Re}(a_n)$ within the context of the current discussion of vector spaces.[5] As we talked about in the last lecture, if we write a vector $\mathbf{v}$ as a linear combination of orthogonal vectors $\mathbf{u}_n$

$$\mathbf{v} = \sum_{n=1}^{N} v_n \mathbf{u}_n \,, \tag{16}$$

then the coefficients v_n in are given by

$$v_n = \frac{(\mathbf{u}_n, \mathbf{v})}{(\mathbf{u}_n, \mathbf{u}_n)} \,. \tag{17}$$

For the example at hand, Eq. (15) is equivalent to Eq. (16), but in order apply Eq. (17) to find the coefficients $\mathrm{Re}(a_n)$ in Eq. (15), we need the definition of the inner product of two vectors for this vector space. For any N dimensional vector space the inner product between two vectors $\mathbf{w}$ and $\mathbf{v}$ can be written as (See Exercise 14.5)

$$(\mathbf{w}, \mathbf{v}) = \begin{pmatrix} w_1^* & w_2^* & \dots & w_N^* \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{pmatrix}, \tag{18}$$

where w_n and v_n are the components of the vectors $\mathbf{w}$ and $\mathbf{v}$ in the same basis. Notice that the elements of the row matrix in Eq. (18) are the complex conjugates of

[4] This is Eq. (10) of the Lecture 10 notes.

[5] Note that Eq. (15) says, at its most basic level, that the eigenvectors [Eq. (13)] form a basis for the space of initial displacements of the objects (which can be any set of N real numbers).

the elements of $\mathbf{u}$. Of course, if we are dealing with real vector, then the complex conjugate is simply the element itself. Note that Eq. (18) can be written in more compact form as

$$(\mathbf{w},\mathbf{v}) = \sum_{j=1}^{N} w_j^* v_j \,. \tag{19}$$

Using the form of the inner product in Eq. (19), the application of Eq. (17) to the coupled oscillator problem is thus[6]

$$\mathrm{Re}(a_n) = \frac{\sum_{j=1}^{N} \sin\left(\frac{n\pi}{N+1} j\right) q_j(0)}{\sum_{j=1}^{N} \sin^2\left(\frac{n\pi}{N+1} j\right)}. \tag{20}$$

III. Vectors Spaces and Fourier Series

The last vector-space example is Fourier Series. Recall, the complex Fourier-series representation of a function $f(x)$ defined on the interval $-L$ to L is

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L} \,, \tag{21a}$$

where the coefficients c_n are given by

$$c_n = \frac{1}{2L} \int_{-L}^{L} f(x) e^{-in\pi x/L}\, dx \,. \tag{21b}$$

If you have been paying attention to this point (i.e, if you are still awake), then you should be thinking "Ah ha! Equation (21) says that we can write the function $f(x)$ as a linear combination of the (basis!) functions $e^{in\pi x/L}$ with coefficients c_n. Looks like a vector space to me! And ah ha, again! It seems that somehow Eq. (21b) is the equivalent of Eq. (17), where the coefficients are expressed in terms of inner products on this space." But likely you are now asleep and thinking about other things.

But if you were awake, you would be entirely correct. Let's see that this is the case. The vectors in this space are indeed functions on the interval $-L$ to L, and one set of

[6] Equation (20) is Eq. (18) of the Lecture 10 notes.

basis vectors $\mathbf{u}_n$ is indeed the set of functions $u_n(x) = e^{in\pi x/L}$, $-\infty < n < \infty$. So what is the inner product on this space that makes these basis vectors orthogonal? You actually saw the inner product back in Lecture 12 before you knew it was an inner product, so let me remind you. Denoting, for example, a function $f(x)$ as the vector $\mathbf{f}$, we define the inner product $(\mathbf{g},\mathbf{f})$ in this space as

$$(\mathbf{g},\mathbf{f}) = \int_{-L}^{L} g^*(x) f(x) dx . \tag{22}$$

Again, note the complex conjugate in the definition. Also notice the similarity of Eqs. (19) and (22). Using Eq. (22), Eq. (21) can be written in vector-space notation as

$$\mathbf{f} = \sum_{n=-\infty}^{\infty} c_n \mathbf{u}_n , \tag{23a}$$

$$c_n = \frac{(\mathbf{u}_n,\mathbf{f})}{(\mathbf{u}_n,\mathbf{u}_n)}. \tag{23b}$$

Lastly, let's revisit the idea of an orthonormal basis within the context of Fourier series. Recall, a normalized (or unit) vector $\hat{\mathbf{u}}$ is defined by $\|\hat{\mathbf{u}}\| = \sqrt{(\hat{\mathbf{u}},\hat{\mathbf{u}})} = 1$, and we can normalize any vector $\mathbf{u}$ via

$$\hat{\mathbf{u}} = \frac{\mathbf{u}}{\sqrt{(\mathbf{u},\mathbf{u})}} . \tag{25}$$

Let's find the normalized version of the basis functions $u_n(x) = e^{in\pi x/L}$. Calculating $(\mathbf{u}_n,\mathbf{u}_n)$ we have

$$(\mathbf{u}_n,\mathbf{u}_n) = \int_{-L}^{L} e^{-in\pi x/L}\, e^{in\pi x/L}\, dx = 2L . \tag{26}$$

We can thus turn our *orthogonal* basis into an *orthonormal* basis by using the normalized vectors

$$\hat{\mathbf{u}}_n = \frac{e^{in\pi x/L}}{\sqrt{2L}}. \tag{27}$$

If we now write a vector in this space as a linear combination of these normalized basis vectors,

$$\mathbf{f} = \sum_{n=-\infty}^{\infty} c_n \hat{\mathbf{u}}_n \,, \tag{28a}$$

$$c_n = (\hat{\mathbf{u}}_n, \mathbf{f}) \tag{28b}$$

then the functional expression of Eq. (28) results in the Fourier series being written as

$$f(x) = \frac{1}{\sqrt{2L}} \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L} \,, \tag{29a}$$

$$c_n = \frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x) e^{-in\pi x/L}\, dx \,. \tag{29b}$$

To some, the Fourier Series written as Eq. (29) is more appealing because it has a certain symmetry that Eq. (21) lacks.

Exercises

***14.1** Consider the operator $A = \begin{pmatrix} i & j \\ k & l \end{pmatrix}$ on a two dimensional vector space. Show that for any two scalars a and b and any two vectors $\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$ and $\mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$ that this operator is linear, i.e., that it satisfies Eq. (2).

***14.2** Show that for any two scalars a and b and any two functions $f(x)$ and $g(x)$, that the differential operator $i\dfrac{d}{dx}$ is linear, i.e., that it satisfies Eq. (2).

***14.3** In solving the $N = 3$ coupled oscillator problem, we found the three eigenvectors to the associated eigenvalue problem, which can be written as

$\mathbf{u}_1 = \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$, $\mathbf{u}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$, and $\mathbf{u}_1 = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$. Find the normalized versions $\hat{\mathbf{u}}_1$, $\hat{\mathbf{u}}_2$, and $\hat{\mathbf{u}}_3$ of each of these vectors.

**14.4 Consider the time independent Schrödinger equation eigenvalue problem $H\psi = E\psi$, where H is the operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2$. This is the (1D) quantum mechanical harmonic-oscillator problem. The solutions (eigenvectors and eigenvalues) of this problem can be written as ($n = 0,1,2,\ldots$)

$$\psi_n(x) = \left(\frac{d}{dx} - ax\right)^n e^{-ax^2/2}, \text{ where } a = \sqrt{mk/\hbar^2} \text{ and}$$

$$E_n = \frac{\hbar\tilde{\omega}}{2} + n\hbar\tilde{\omega}, \text{ where } \tilde{\omega} = \sqrt{k/m}$$

(**a**) For $n = 0$ (the ground state), show that $\psi_0(x)$ is a solution to $H\psi = E\psi$ with the appropriate eigenvalue.
(**b**) For this vector space, the inner product of two vectors $\boldsymbol{\psi}$ and $\boldsymbol{\varphi}$ is defined as $(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \int_{-\infty}^{\infty} \varphi^*(x)\psi(x)dx$. Show that the $n = 0$ and $n = 1$ states are orthogonal.
(**c**) Find the norm of the $n = 0$ state. Thus construct the normalized eigenvector corresponding to this state.
(**d**) Given that $H\psi_0 = E_0\psi_0$ and $H\psi_1 = E_1\psi_1$, find $H\varphi$, where $\varphi = C_0\psi_0 + C_1\psi_1$ (Here $C_0 \neq 0$ and $C_1 \neq 0$ are two constants.) Thus argue that the wave function φ is *not* an eigenvector of H (for any value of E).

*14.5 **Inner product**. Consider two vectors written in terms of some orthonormal basis,

$$\mathbf{v} = \sum_{n=1}^{N} v_n \mathbf{u}_n, \quad \mathbf{w} = \sum_{m=1}^{N} w_m \mathbf{u}_m.$$

(**a**) Using Eq. (10) of the Lecture 13 notes, show that the inner product $(\mathbf{w}, \mathbf{v})$ can be expressed in terms of the components of the two vectors as $(\mathbf{w}, \mathbf{v}) = \sum_{n=1}^{N} w_n^* v_n$.

(**b**) What is the norm of the vector $\mathbf{v}$ expressed in terms of its components?

*__14.6 Inner Product and Fourier Series__. Consider two functions expressed as their normalized Fourier Series representations,

$$f(x)=\frac{1}{\sqrt{2L}}\sum_{n=-\infty}^{\infty}c_n e^{in\pi x/L}\ ,\ g(x)=\frac{1}{\sqrt{2L}}\sum_{m=-\infty}^{\infty}d_n e^{im\pi x/L}\ .$$

(**a**) Starting with these expressions, show that the inner product $(\mathbf{g},\mathbf{f})=\int_{-L}^{L}g^*(x)f(x)dx$ can be expressed in terms of the Fourier coefficients c_n and d_n as $(\mathbf{g},\mathbf{f})=\sum_{n=-\infty}^{\infty}d_n^*c_n$.

(**b**) What is the norm of $f(x)$ in terms of its Fourier coefficients?

Notice the similarity of these results and those of Exercise 14.5. Cool, eh?

The Dirac Delta Function

Overview and Motivation: The Dirac delta function is a concept that is useful throughout physics. For example, the charge density associated with a point charge can be represented using the delta function. As we will see when we discuss Fourier transforms (next lecture), the delta function naturally arises in that setting.

Key Mathematics: The Dirac delta function!

I. Introduction

The basic equation associated with the **Dirac delta function** $\delta(x)$ is

$$\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0), \tag{1}$$

where $f(x)$ is any function that is continuous at $x = 0$. Equation (1) should seem strange: we have an integral that only depends upon the value of the function $f(x)$ at $x = 0$. Because an integral is "the area under the curve," we expect its value to not depend only upon one particular value of x. Indeed, there is no function $\delta(x)$ that satisfies Eq. (1). However, there is another kind of mathematical object, known as a *generalized function* (or *distribution*), that can be defined that satisfies Eq. (1).

A **generalized function** can be defined as the limit of a sequence of functions. Let's see how this works in the case of $\delta(x)$. Let's start with the normalized Gaussian functions

$$g_n(x) = \sqrt{\frac{n}{\pi}} e^{-nx^2}. \tag{2}$$

Here $n = 1/\sigma^2$, where σ is the standard Gaussian width parameter. These functions are normalized in the sense that their integrals equal 1,

$$\int_{-\infty}^{\infty} g_n(x) dx = 1 \tag{3}$$

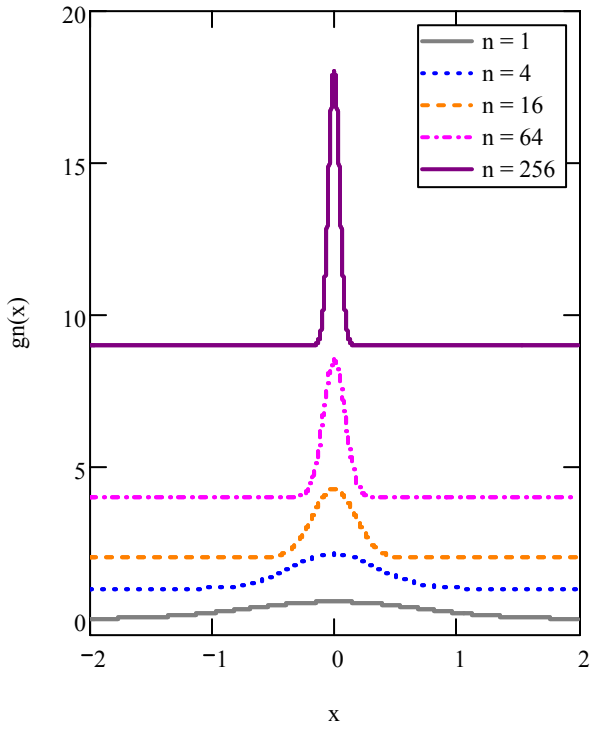
for any value of n (>0). Let's now consider the sequence of functions for $n = 1, 2, 3, \ldots$,

$$g_1(x)=\sqrt{\frac{1}{\pi}}e^{-x^2},\ g_2(x)=\sqrt{\frac{2}{\pi}}e^{-2x^2},\ \ldots,\ g_{100}(x)=\sqrt{\frac{100}{\pi}}e^{-100x^2},\ \ldots \tag{4}$$

What does this sequence of functions look like? We can summarize this sequence as follows. As n increases

(a) $g_n(0)$ becomes larger;
(b) $g_n(x\neq 0)$ eventually becomes smaller;
(c) the width of the center peak becomes smaller;
(d) but $\int_{-\infty}^{\infty} g_n(x)dx=1$ remains constant.

The following figure plots some of the functions in this sequence.



Let's now ask ourselves, what does the $n=\infty$ limit of this sequence look like? Based on (a) through (d) above we would (perhaps simplistically) say

(a) $g_\infty(0)=\infty$;
(b) $g_n(x\neq 0)=0$;
(c) the width of the center peak equals zero;

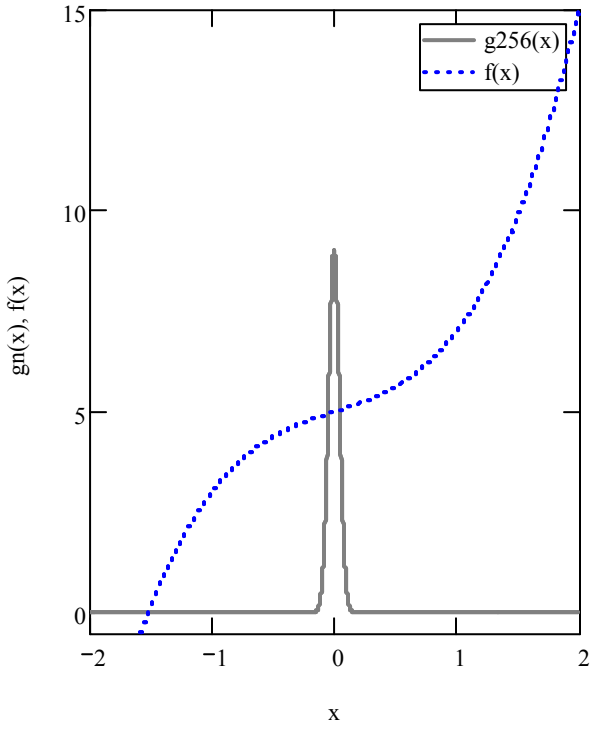
(d) but $\int_{-\infty}^{\infty} g_\infty(x)dx = 1$.

Note that (a) and (b) are not compatible with (d) if $g_\infty(x)$ is a function in the standard sense, because for a function (a) and (b) would imply that the integral of $g_\infty(x)$ is zero.

So how should we think of this sequence of functions, then? Well, the sequence is only really useful if it appears as part of an integral, as in, for example,

$$\lim_{n\to\infty}\int_{-\infty}^{\infty} g_n(x)f(x)dx = \lim_{n\to\infty}\int_{-\infty}^{\infty}\sqrt{\tfrac{n}{\pi}}e^{-nx^2}f(x)dx. \tag{5}$$

Let's calculate the integral, and then the limit in Eq. (5). The following figure should help with the calculation.



As n get large, $g_n(x) = \sqrt{\tfrac{n}{\pi}}e^{-nx^2}$ becomes narrower such that it only has weight very close to $x = 0$. Thus, as far as the integral is concerned, for large enough n only $f(x)$ at $x = 0$ is important. We can thus replace $f(x)$ by $f(0)$ in the integral, which gives us

$$\lim_{n\to\infty}\int_{-\infty}^{\infty}\sqrt{\tfrac{n}{\pi}}e^{-nx^2}\ f(x)dx = f(0)\lim_{n\to\infty}\int_{-\infty}^{\infty}\sqrt{\tfrac{n}{\pi}}e^{-nx^2}\ dx = f(0)\lim_{n\to\infty}1 = f(0) \tag{6}$$

Thus, the integral on the lhs of Eq. (1) is really shorthand for the integral on the lhs of Eq. (6), That is, the Dirac delta function is defined via the equation

$$\int_{-\infty}^{\infty}\delta(x)f(x)dx = \lim_{n\to\infty}\int_{-\infty}^{\infty}\sqrt{\tfrac{n}{\pi}}e^{-nx^2}\ f(x)dx \tag{7}$$

Now often (as physicists) we often get lazy and write

$$\delta(x) = \lim_{n\to\infty}\sqrt{\tfrac{n}{\pi}}e^{-nx^2}, \tag{8}$$

but this is simply shorthand for Eq. (7). Eq. (8) really has no meaning unless the function $\sqrt{\frac{n}{\pi}}e^{-nx^2}$ appears *inside* an integral and the limit $\lim_{n\to\infty}$ appears *outside* the same integral. However, after you get used to working with the delta function, you will rarely need to even think about the limit that is used to define it.

One other thing to note. This particular sequence of functions $g_n(x) = \sqrt{\frac{n}{\pi}}e^{-nx^2}$ that we have used here is not unique. There are infinitely many sequences that can be used to define the delta function. For example, we could also have defined $\delta(x)$ via

$$\delta(x) = \lim_{n\to\infty}\frac{1}{\pi}\frac{\sin(nx)}{x}. \tag{9}$$

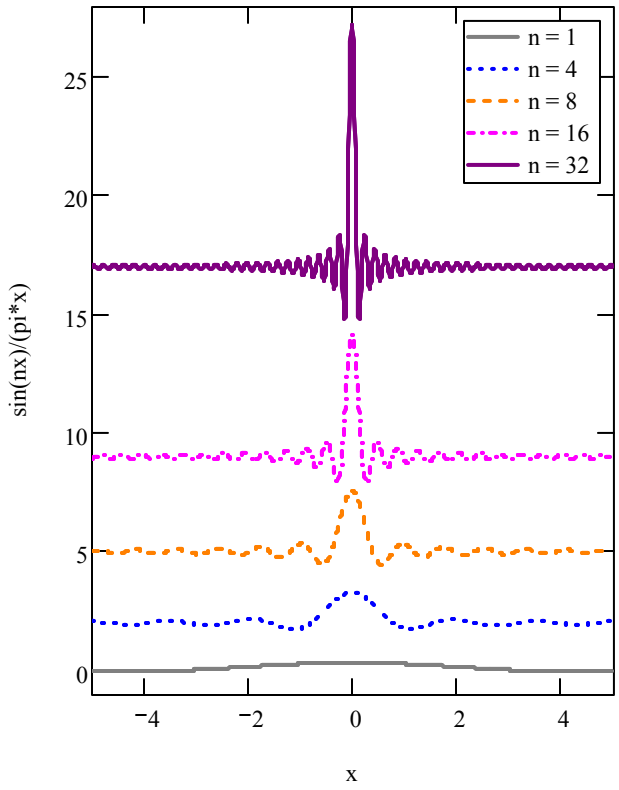
The sequence of functions $\sin(nx)/(\pi x)$ is illustrated in the figure at the top of the next page.

Notice that the key features of both of these two difference sequences are expressed by (a) – (d) at the top of page 5.

II. Delta Function Properties

There are a number of properties of the delta function that are worth committing to memory. They include the following,

$$\int_{-\infty}^{\infty}\delta(x-x')f(x)dx = f(x'), \tag{10}$$



$$\int_{-\infty}^{\infty} \delta'(x) f(x) dx = -f'(0) \tag{11}$$

$$\delta(x/a) = |a| \delta(x) \tag{12}$$

The proof of Eq. (10) is relatively straightforward. Let's change the integration variable to $y = x - x'$, $dy = dx$, which gives

$$\int_{-\infty}^{\infty} \delta(x - x') f(x) dx = \int_{-\infty}^{\infty} \delta(y) f(y + x') dy \,. \tag{13}$$

Then using Eq. (1), we see that Eq. (10) is simply equal to $f(x')$. *QED*.

Let's also prove Eq. (12). We do this in two steps, for $a > 0$ and then for $a < 0$.
(*i*) First, we assume that $a > 0$. Then

$$\int_{-\infty}^{\infty}\delta(x/a)dx=\int_{-\infty}^{\infty}\delta\left(x/|a|\right)dx \tag{14}$$

Changing integration variable $y=x/|a|$, $dy=dx/|a|$, this last equation becomes

$$\int_{-\infty}^{\infty}\delta(x/a)dx=|a|\int_{-\infty}^{\infty}\delta(y)dy \tag{15}$$

and changing variables back to x via $x=y$, $dx=dy$ gives

$$\int_{-\infty}^{\infty}\delta(x/a)dx=|a|\int_{-\infty}^{\infty}\delta(x)dx \tag{16}$$

and so for $a>0$ we have $\delta(x/a)=|a|\delta(x)$.

(*ii*) We now assume $a<0$. Then we have

$$\int_{-\infty}^{\infty}\delta(x/a)dx=\int_{-\infty}^{\infty}\delta\left(-x/|a|\right)dx \tag{17}$$

Changing integration variable $y=-x/|a|$, $dy=-dx/|a|$, this last equation becomes

$$\begin{aligned}\int_{-\infty}^{\infty}\delta(x/a)dx&=-|a|\int_{\infty}^{-\infty}\delta(y)dy\\&=|a|\int_{-\infty}^{\infty}\delta(y)dy\\&=|a|\int_{-\infty}^{\infty}\delta(x)dx\end{aligned} \tag{18}$$

and so for $a<0$ we also have $\delta(x/a)=|a|\delta(x)$. *QED*.

We leave the proof of Eq. (11) as an exercise.

III. Fourier Series and the Delta Function

Recall the complex Fourier series representation of a function $f(x)$ defined on $-L \le x \le L$,

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L}, \tag{19a}$$

$$c_n = \frac{1}{2L}\int_{-L}^{L} f(x) e^{-in\pi x/L}\, dx. \tag{19b}$$

Let's now substitute c_n from Eq. (19b) into Eq. (19a). Before we do this we must change the variable x in either Eq. (19a) or (19b) to something else because the variable x in Eq. (19b) is just a (dummy) integration variable. Changing x to x' in Eq. (19a) and doing the substitution we end up with

$$f(x') = \sum_{n=-\infty}^{\infty}\left(\frac{1}{2L}\int_{-L}^{L} f(x) e^{-in\pi x/L}\, dx\right) e^{in\pi x'/L} \tag{20}$$

Let's now switch the integration and summation (assuming that this is OK to do). This produces

$$f(x') = \int_{-L}^{L}\left[\frac{1}{2L}\sum_{n=-\infty}^{\infty} e^{in\pi(x'-x)/L}\right] f(x)\, dx \tag{21}$$

If we now compare Eq. (21) to Eq. (10), we see that we can identify another representation of the delta function

$$\delta(x-x') = \frac{1}{2L}\sum_{n=-\infty}^{\infty} e^{in\pi(x'-x)/L} \tag{22}$$

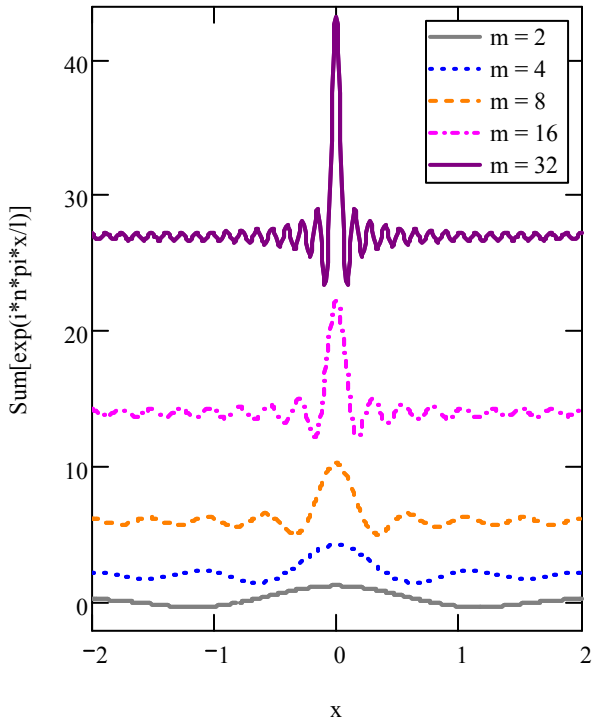
or setting $x' = 0$ we have

$$\delta(x) = \frac{1}{2L}\sum_{n=-\infty}^{\infty} e^{-in\pi x/L} \tag{23}$$

So how is this equation related to the delta function being defined as the limit of a sequence of functions? Well, we can re-express Eq. (23) as a sequence of functions via

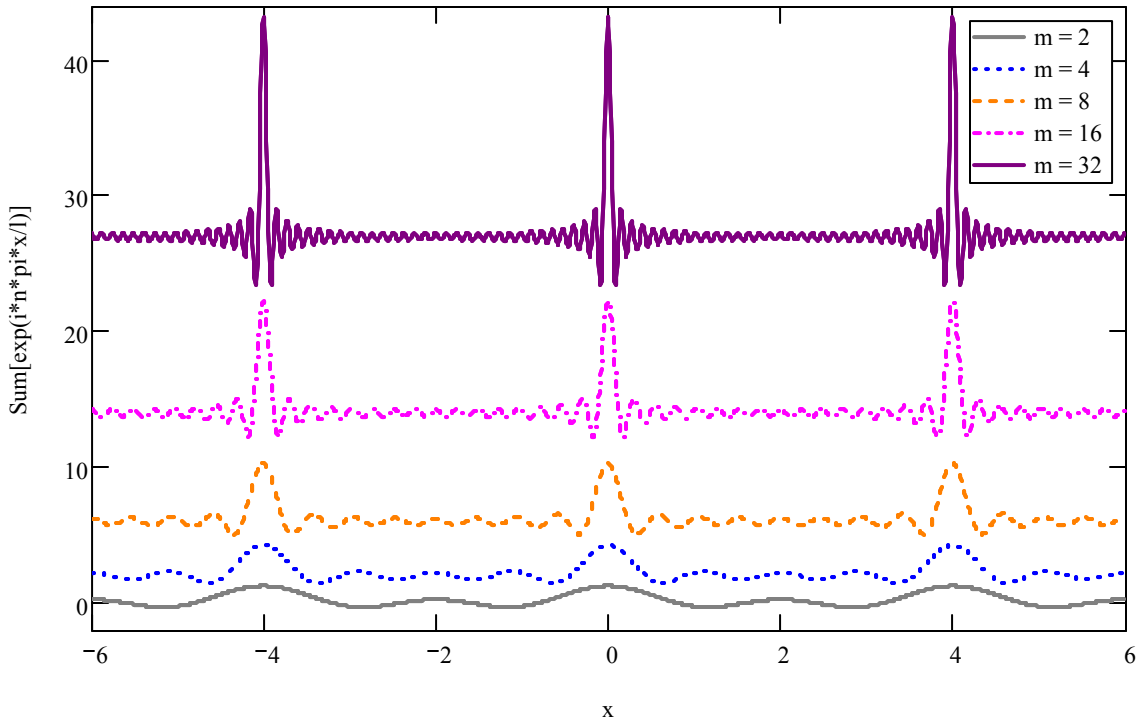
$$\delta(x) = \lim_{m\to\infty} \frac{1}{2L} \sum_{n=-m}^{m} e^{-in\pi x/L} \,. \tag{24}$$

The following figure plots $\frac{1}{2L}\sum_{n=-m}^{m} e^{-in\pi x/L}$ for several values of m (for $L = 2$). Notice that these functions are quite similar to the function $\sin(mx)/(\pi x)$ plotted above.[1]



However, there is one important difference between these two sequences of functions. Because the functions $e^{-in\pi x/L}$ that appear in the sum in Eqs. (23) and (24) all repeat with on an interval of length $2L$, Eq. (24) is actually a series of delta functions, centered at $x = 0, \pm 2L, \pm 4L, \pm 6L, \ldots$. This is illustrated in the next figure, where we have expanded the x axis beyond the limits of $-L$ to L. Thus, the equality expressed by Eq. (23) or (24) is only valid on the interval $-L \le x \le L$.

[1] We have changed the n to m in the $\sin(nx)/(\pi x)$ functions because we are now using m to label the functions in the sequence.



Exercises

*__15.1__ Equation (11), $\int_{-\infty}^{\infty} \delta'(x) f(x) dx = -f'(0)$, can be taken as the definition of the derivative of the delta function. Treating the delta function as a normal function, show that Eq. (11) is true. (Hint: use integration by parts.)

*__15.2__ Show that the equation $\delta(x) = \lim_{m\to\infty} \frac{1}{2L} \sum_{n=-m}^{m} e^{-in\pi x/L}$ can be re-expressed as $\delta(x) = \lim_{m\to\infty} \frac{1}{2L} \sum_{n=-m}^{m} \cos\left(\frac{n\pi x}{L}\right)$. This is perhaps more appealing because the delta function is a real function and the rhs is now explicitly real.

*__15.3__ Find another sequence of functions, not based on either the Gaussian or $\sin(x)/x$ functions, that has as its limit the delta function.

Introduction to Fourier Transforms

Overview and Motivation: Fourier transform theory is the extension of Fourier series theory to functions that are defined for all values of x. Thus, we will be able to represent a function defined for $-\infty \le x \le \infty$ as a linear combination of harmonic functions.

Key Mathematics: Fourier transforms and more vector-space theory.

I. Fourier Series vs the Fourier Transform

By now you should be intimately familiar with the Fourier series representation of a function $f(x)$ on the interval $-L \le x \le L$. A representation that uses the normalized harmonic functions $\frac{1}{\sqrt{2L}} e^{in\pi x/L}$ (introduced in Lecture 14) is

$$f(x) = \frac{1}{\sqrt{2L}} \sum_{n=-\infty}^{\infty} c_n e^{in\pi x/L}, \tag{1a}$$

$$c_n = \frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x) e^{-in\pi x/L}\, dx. \tag{1b}$$

As we know the Fourier series representation is useful for any function that we only need to define within the bounds $-L \le x \le L$. Outside that interval, the representation is periodic with period $2L$ because the rhs of Eq. (1a) has a period of $2L$.

There are many times, however, when we wish to represent a (nonperiodic) function on the entire real line as a linear combination of harmonic functions. To do this we can take the $L \to \infty$ limit of Eq. (1). This limit (which we will not go through, but is well defined) yields the following pair of relationships

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

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

There are several things to notice about Eq. (2). First, we have traded in the discrete index n in Eq. (1) for the continuous variable $k = (n\pi/L)(= 2\pi/\lambda)$, which is already familiar as the wave vector. Second, if we compare Eqs. (1) and (2), we might conclude that $\frac{1}{\sqrt{2\pi}} e^{ikx}$ are now our normalized harmonic functions. That is correct, as we discuss in further detail below. With that, we can then interpret the function $h(k)$ as the coefficient (or component) of the harmonic function $\frac{1}{\sqrt{2\pi}} e^{ikx}$. This function $h(k)$ has a special name: it is known as the **Fourier transform** of the function $f(x)$. The Fourier transform $h(k)$ is thus analogous to the Fourier coefficients c_n that appear in the Fourier series. The other feature of Eq. (2) that you undoubtedly noticed is that $f(x)$ is expressed as a continuous sum (integral) over basis functions rather than a discrete sum over basis functions. This is a necessary consequence of the $L \to \infty$ limit.

Because of the resultant symmetry in the two relationships in Eq. (2), the function $f(x)$ is also known as the **inverse Fourier transform** of $h(k)$. In fact, because $f(x)$ and $h(k)$ are obtainable from each other, they each contain the same information, just in a different form.[1]

We remark that there are technical criteria that the function $f(x)$ must meet for Eq. (2) to be valid. A sufficient condition is that $f(x)$ be square integrable,

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx < \infty . \tag{3}$$

If Eq. (3) is true, then $h(k)$ is also square integrable and it can be shown that

$$\int_{-\infty}^{\infty} |f(x)|^2 \, dx = \int_{-\infty}^{\infty} |h(k)|^2 \, dk \tag{4}$$

The proof of Eq. (4) is left as an exercise.

II. The Fourier Transform and Vector Space Theory

As we also discussed in Lecture 14, the Fourier series [Eq. (1)] can be thought of as a pair of vector-space relationships

[1] Of course, the same is true about the function $f(x)$ and the coefficients c_n in the Fourier series. Knowing the c_n's is equivalent to knowing the function $f(x)$ itself.

$$\mathbf{f} = \sum_{n=-\infty}^{\infty} c_n \hat{\mathbf{u}}_n \,, \tag{5a}$$

$$c_n = (\hat{\mathbf{u}}_n, \mathbf{f}) \tag{5b}$$

where the vector $\mathbf{f}$ is the function $f(x)$, $\hat{\mathbf{u}}_n = \frac{1}{\sqrt{2L}} e^{in\pi x/L}$ is an orthonormal basis vector, c_n is the corresponding component of $\mathbf{f}$, and the inner product is defined as

$$(\mathbf{g}, \mathbf{f}) = \int_{-L}^{L} g^*(x) f(x) dx \,. \tag{6}$$

Further, because the basis functions are orthonormal, we have the relationship for their inner product

$$(\hat{\mathbf{u}}_m, \hat{\mathbf{u}}_n) = \delta_{mn} \,, \tag{7}$$

where δ_{mn}, known as the **Kronecker delta**, equals 1 if $m = n$ and equals 0 otherwise. Eq. (7) is the standard way of expressing the orthonormality of the basis vectors.

We now want to put Fourier-transform theory on the same vector-space footing as Fourier series. This is actually fairly straightforward, except that there is a bit of subtlety needed in defining the inner product, as we shall see. First, if we identify the basis vectors as the harmonic functions[2]

$$\hat{u}(k, x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \,, \tag{8}$$

then Eq. (2) can be written as

$$f(x) = \int_{-\infty}^{\infty} h(k) \hat{u}(k, x) dk \,, \tag{9a}$$

$$h(k) = \int_{-\infty}^{\infty} \hat{u}^*(k, x) f(x) \, dx \tag{9b}$$

[2] To keep the notation as simple as possible, we drop the formal vector notation and just use the functional form of the vectors for this space.

A comparison of Eqs. (5) and (9) then suggests that we define the inner product on this vector space as

$$\left(g(x), f(x)\right) = \int_{-\infty}^{\infty} g^*(x) f(x) dx \tag{10}$$

Let's see what this gives us if we calculate $\left(\hat{u}(k',x), \hat{u}(k,x)\right)$ for this vector space. If life is good then we expect to get $\left(\hat{u}(k',x), \hat{u}(k,x)\right) = \delta_{k'k}$, similar to Eq. (7). Let's see what happens. Using Eq. (10) we have

$$\left(\hat{u}(k',x), \hat{u}(k,x)\right) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx \tag{11}$$

We consider two cases separately, $k = k'$ and $k \neq k'$.
(*i*) If $k = k'$, then Eq. (11) integrates to

$$\left(\hat{u}(k,x), \hat{u}(k,x)\right) = \frac{1}{2\pi} x\Big|_{-\infty}^{\infty}, \tag{12a}$$

which is undefined. Hum… Not too good. Let's look at the other case.
(*ii*) If $k \neq k'$, then Eq. (11) integrates to

$$\left(\hat{u}(k,x), \hat{u}(k,x)\right) = \frac{1}{2\pi} \frac{1}{i(k-k')} e^{i(k-k')x}\Big|_{-\infty}^{\infty} \tag{12b}$$

Unfortunately, this is not defined either! So it looks like either the basis functions or the inner product is unsuitable.

As it turns out, we can fix this dilemma by defining the inner product slightly differently as

$$\left(g(x), f(x)\right) = \lim_{n\to\infty} \int_{-\infty}^{\infty} e^{-x^2/n}\, g^*(x) f(x) dx\,. \tag{13}$$

Notice what the function $e^{-x^2/n}$ does for us. For any finite n this Gaussian function cuts off the integrand fast enough to make the integral converge. Furthermore in the limit $n \to \infty$ the function itself simply approaches 1.[3]

Let's see what happens with this definition of the inner product. We now have

$$\left(\hat{u}(k',x),\hat{u}(k,x)\right) = \frac{1}{2\pi}\lim_{n\to\infty}\int_{-\infty}^{\infty} e^{-x^2/n}\; e^{i(k-k')x}dx\,. \tag{14}$$

To take advantage of the symmetry of the Gaussian we rewrite this as

$$\left(\hat{u}(k',x),\hat{u}(k,x)\right) = \frac{1}{2\pi}\lim_{n\to\infty}\int_{-\infty}^{\infty} e^{-x^2/n}\; \{\cos[(k-k')x]+i\sin[(k-k')x]\}dx\,. \tag{15}$$

Because $e^{-x^2/n}$ is even, the integral involving the sine function is zero, so this simplifies to

$$\left(\hat{u}(k',x),\hat{u}(k,x)\right) = \frac{1}{2\pi}\lim_{n\to\infty}\int_{-\infty}^{\infty} e^{-x^2/n}\; \cos[(k-k')x]dx\,. \tag{15}$$

We have seen this integral before (see Lecture 12). Calculating the integral, Eq. (15) becomes

$$\left(\hat{u}(k',x),\hat{u}(k,x)\right) = \frac{1}{2}\lim_{n\to\infty}\sqrt{\tfrac{n}{\pi}}\,e^{-n(k-k'/2)^2} \tag{16}$$

Now you may remember from the last lecture that the limit of a similar sequence of Gaussian functions is the Dirac delta function. If you closely compare Eq. (16) with Eq. (8) from the Lecture 15 notes, you will see that Eq. (16) can be expressed as

$$\left(\hat{u}(k',x),\hat{u}(k,x)\right) = \frac{1}{2}\,\delta\left(\frac{k-k'}{2}\right) \tag{17}$$

And using the relationship $\delta(x/a) = |a|\,\delta(x)$, this simplifies to

[3] In fact, $\lim_{n\to\infty} e^{-x^2/n}$ is one definition of the unit distribution.

$$\left(\hat{u}(k',x),\hat{u}(k,x)\right)=\delta(k-k') \tag{18}$$

This, then, is the **orthogonality relationship** for the basis functions $\hat{u}(k,x)=\frac{1}{\sqrt{2\pi}}e^{ikx}$. Notice that it is similar to Eq. (7) for the Fourier series basis functions, but instead of the Krocecker delta, we have the Dirac delta function. That the orthogonality relationship is a distribution rather than a simple function is a result of the variable k being continuous rather than discrete.

You will often see written

$$\delta(k-k')=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i(k-k')x}\,dx\,, \tag{19}$$

but this is really shorthand for the limiting procedure that we did above. That is, it is really shorthand for

$$\delta(k-k')=\frac{1}{2\pi}\lim_{n\to\infty}\int_{-\infty}^{\infty}e^{-x^2/n}\,e^{i(k-k')x}\,dx\,. \tag{20}$$

Note that Eq. (20) is a definition of the delta function as the limit of a sequence of functions (which is exactly equivalent to our original definition using the sequence of Gaussian functions).

Now that we have the inner product suitably defined, let go back to the Fourier transform equation and see that $h(k)$ is indeed equal to the inner product $\left(\hat{u}(k,x),f(x)\right)$. So using Eq. (13) we calculate the inner product of $\hat{u}(k,x)$ with Eq. (2a)[4]

$$\left(\hat{u}(k,x),f(x)\right)=\lim_{n\to\infty}\int_{-\infty}^{\infty}e^{-x^2/n}\,\frac{1}{\sqrt{2\pi}}e^{-ikx}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}h(k')e^{ik'x}\,dk'\right]dx \tag{21}$$

If we switch the order of integration in this equation we get something that should look familiar,

[4] Notice that we have renamed the integration variable on the rhs of Eq. (2a) because we have another variable k in this equation.

$$\left(\hat{u}(k,x), f(x)\right) = \frac{1}{2\pi} \lim_{n\to\infty} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} e^{-x^2/n}\, e^{i(k'-k)x}\, dx \right] h(k')dk' \tag{22}$$

But from Eq. (20) we see that Eq. (22) is simply

$$\left(\hat{u}(k,x), f(x)\right) = \int_{-\infty}^{\infty} \delta(k'-k)h(k')dk', \tag{23}$$

which gives us the result that we want,

$$\left(\hat{u}(k,x), f(x)\right) = h(k). \tag{24}$$

Thus, as with the c_n's in the Fourier series representation of a function, the Fourier transform $h(k)$ can be though of as the inner product of the normalized basis function with the original function $f(x)$.

Exercises

*__16.1__ Show that Eq. (4), $\int_{-\infty}^{\infty} |f(x)|^2\, dx = \int_{-\infty}^{\infty} |h(k)|^2\, dk$, is true.

*__16.2__ Calculate the Fourier transform of the function $f(x) = e^{-|x|}$. Plot the resulting function vs k.

**__16.3__ As the notes discuss, the original attempt at defining the inner product as $\left(g(x), f(x)\right) = \int_{-\infty}^{\infty} g^*(x) f(x) dx$ needs to be slightly modified. We chose one particular way that this can be done. Another choice that we could have made is $\left(g(x), f(x)\right) = \lim_{n\to\infty} \int_{-n}^{n} g^*(x) f(x) dx$. Show that this definition of the inner product also gives the result $\left(\hat{u}(k',x), \hat{u}(k,x)\right) = \delta(k-k')$ for the inner product of two basis functions. {Hint: you will need to use the second definition of the delta function from Lecture 15 [Eq. (9) on p. 4]}.

Fourier Transforms and the Wave Equation

Overview and Motivation: We first discuss a few features of the Fourier transform (FT), and then we solve the initial-value problem for the wave equation using the Fourier transform.

Key Mathematics: More Fourier transform theory, especially as applied to solving the wave equation.

I. FT Change of Notation

In the last lecture we introduced the FT of a function $f(x)$ through the two equations

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

$$\hat{f}(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-ikx}\,dx\,. \tag{1b}$$

Note that we have changed notation compared to the last lecture. Hereafter we designate the FT of any function by the same symbol, but with an overhead caret included. That is, the FT of $f(x)$ we now write as $\hat{f}(k)$. As we shall see, this is useful when dealing with equations that include FTs of several functions. [1]

II. Some Properties of the Fourier Transform

We now discuss several useful properties of the Fourier transform.

A. Translation

The first property has to do with translation of the function $f(x)$. Let's say we are interested in $f(x-x_0)$, which corresponds to translation of $f(x)$ by x_0. Then, using Eq. (1a) we can write

$$\begin{aligned} f(x-x_0)&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{f}(k)e^{ik(x-x_0)}\,dk \\ &=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\hat{f}(k)e^{-ikx_0}\right]e^{ikx}\,dk \end{aligned} \tag{2}$$

[1] This notation is fairly common practice. At some point you may even see the FT of $f(x)$ written as $f(k)$. At least we won't be doing that here!

Thus, we see that the FT of $f(x-x_0)$ is $\hat{f}(k)e^{-ikx_0}$. In other words, translation of $f(x)$ by x_0 corresponds to multiplying the FT $\hat{f}(k)$ by e^{-ikx_0}.

B. Differentiation

The second property has to do with the FT of $f'(x)$, the derivative of $f(x)$. Again, using Eq. (1a) we have

$$f'(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[ik\,\hat{f}(k)\right]e^{ikx}\,dk\,. \tag{3}$$

So we see that FT of $f'(x)$ is $ik\,\hat{f}(k)$. That is, differentiation of $f(x)$ corresponds to multiplying $\hat{f}(k)$ by ik.

C. Integration

Let's consider the definite integral of $f(x)$,

$$\int_{x_1}^{x_2}dx\,f(x)=\frac{1}{\sqrt{2\pi}}\int_{x_1}^{x_2}dx\left[\int_{-\infty}^{\infty}dk\,\hat{f}(k)e^{ikx}\right]. \tag{4}$$

Switching the order of integration on the rhs produces

$$\begin{aligned}\int_{x_1}^{x_2}dx\,f(x)&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,\hat{f}(k)\left[\int_{x_1}^{x_2}dx\,e^{ikx}\right]\\&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,\frac{\hat{f}(k)}{ik}\left(e^{ikx_2}-e^{ikx_1}\right)\end{aligned}\,. \tag{5}$$

So if we define $If(x)$ to be the indefinite integral of $f(x)$, we can rewrite Eq. (5) as

$$If(x_2)-If(x_1)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,\frac{\hat{f}(k)}{ik}\left(e^{ikx_2}-e^{ikx_1}\right) \tag{6}$$

So integration of $f(x)$ essentially corresponds to dividing the Fourier transform $\hat{f}(k)$ by ik.[2]

D. Convolution

The last property concerning the a function and its FT has to do with convolution. Because you may not be familiar with convolution, let's first define it. Simply put, the convolution of two functions $f(x)$ and $g(x)$, which we denote $(f*g)(x)$, is defined as

$$(f*g)(x)=\int_{-\infty}^{\infty} f(x-x')g(x')dx' \tag{7}$$

Perhaps the most common place that convolution arises is in spectroscopy, where $g(x)$ is some intrinsic spectrum that is being measured, and $f(x)$ is the resolution function of the spectrometer that is being used to measure the spectrum.[3] The convolution $(f*g)(x)$ is the spectrum that is then measured.

Note that $(f*g)(x)$ is indeed a function of x, and so we can calculate its FT, which we denote $(f\hat{*}g)(k)$. Using Eq. (1b) we can write

$$(f\hat{*}g)(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\left[\int_{-\infty}^{\infty} dx' f(x-x')g(x')\right]e^{-ikx}, \tag{8}$$

which can be rearranged as

$$(f\hat{*}g)(k)=\int_{-\infty}^{\infty} dx' g(x')\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx' f(x-x')e^{-ikx}\right]. \tag{9}$$

Now the quantity in brackets is the FT of $f(x)$ translated by x'. From Sec. II.*B* above we know that this is $\hat{f}(k)e^{-ikx'}$, and so Eq. (9) can be expressed as

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[2] You might think that Eq. (6) could be simplified to $If(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\,\frac{\hat{f}(k)}{ik}e^{ikx}$, but this cannot be done because indefinite integration produces an undetermined integration constant. The constant does not appear in Eq. (6) because it is an equation for the difference of $If(x_2)$ and $If(x_1)$.

[3] The resolution function is often quite close to a Gaussian of a particular, fixed width.

$$(f \hat{*} g)(k) = \hat{f}(k) \int_{-\infty}^{\infty} dx'\, g(x') e^{-ikx'} . \tag{10}$$

Recognizing the integral as $\sqrt{2\pi}\hat{g}(k)$ we finally have

$$(f \hat{*} g)(k) = \sqrt{2\pi}\, \hat{f}(k)\hat{g}(k). \tag{11}$$

So we see that the FT of the convolution is the product of the FT's of the individual functions (along with a factor of $\sqrt{2\pi}$). One way you may hear this result expressed is that convolution in real space (x) corresponds to multiplication in k space. Equation (11) is known as the **convolution theorem**.

III. Solution to the Wave Equation Initial Value Problem

Way back in Lecture 8 we discussed the initial value problem for the wave equation

$$\frac{\partial^2 q(x,t)}{\partial t^2} = c^2 \frac{\partial^2 q(x,t)}{\partial x^2} \tag{12}$$

on the interval $-\infty < x < \infty$. For the initial conditions

$$q(x,0) = a(x), \tag{13a}$$

$$\frac{\partial q}{\partial t}(x,0) = b(x), \tag{13b}$$

we found that the solution to Eq. (12) can be written as

$$q(x,t) = \frac{1}{2}\left[a(x+ct) + a(x-ct) + \frac{1}{c}\int_{x-ct}^{x+ct} b(x')dx' \right]. \tag{14}$$

With the help of the Fourier transform we are now going to rederive this solution, and along the way we will learn something very interesting about the FT of $q(x,t)$.

We start by defining the (spatial) FT of $q(x,t)$ as

$$\hat{q}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} q(x,t) e^{-ikx}\, dx , \tag{15a}$$

so that we also have

$$q(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{q}(k,t)e^{ikx}\,dk\,. \tag{15b}$$

We also define the FT of Eq. (13), the initial conditions,

$$\hat{q}(k,0)=\hat{a}(k), \tag{16a}$$

$$\frac{\partial\hat{q}}{\partial t}(k,0)=\hat{b}(k). \tag{16b}$$

Now each side of the Eq. (12) is a function of x and t, so we can calculate the FT of both sides of Eq (12),

$$\int_{-\infty}^{\infty}\frac{\partial^2 q(x,t)}{\partial t^2}e^{-ikx}dx=c^2\int_{-\infty}^{\infty}\frac{\partial^2 q(x,t)}{\partial x^2}e^{-ikx}dx \tag{17}$$

On the lhs of this equation we can pull the time derivative outside the integral. The lhs is then just the second time derivative of $\hat{q}(k,t)$. The rhs can be simplified by remembering that the FT of the (x) derivative of a function is ik times the FT of the original function. Thus the FT of $\partial^2 q(x,t)/\partial x^2$ is just $-k^2$ times $\hat{q}(k,t)$, the FT of $q(x,t)$. Thus we can rewrite Eq. (17) as

$$\frac{\partial^2\hat{q}(k,t)}{\partial t^2}=-k^2c^2\hat{q}(k,t) \tag{18}$$

This equation should look very familiar to you. What equation is it? None other than the harmonic oscillator equation! What does this tell us about $\hat{q}(k,t)$? It tells us that $\hat{q}(k,t)$ (for a fixed value of k) oscillates harmonically at the frequency $\omega=kc$. Thus we can interpret the function $\hat{q}(k,t)$ as the set of normal modes coordinates for this problem. This further means that the FT has decoupled the equations of motion for this system [as represented by Eq. (12), the wave equation.] Notice also that the dispersion relation $\omega=kc$ has also fallen into our lap by considering the FT of Eq. (12).

As we should know by this point, the solution to Eq. (18) can be written as

$$\hat{q}(k,t)=A(k)e^{ikct}+B(k)e^{-ikct}\,, \tag{19}$$

where $A(k)$ and $B(k)$ are functions of k. And as you should suspect, these two functions are determined by the initial conditions, as follows. First, setting $t=0$ in Eq. (19) and using Eq. (16a) produces

$$\hat{a}(k)=A(k)+B(k), \tag{20a}$$

and calculating the time derivative of Eq. (19), setting $t=0$, and using Eq. (16b) gives us

$$\frac{\hat{b}(k)}{ikc}=A(k)-B(k) \tag{20b}$$

We can solve Eqs. (20a) and (20b) for $A(k)$ and $B(k)$ by taking their sum and difference, which yields

$$A(k)=\frac{1}{2}\left[\hat{a}(k)+\frac{\hat{b}(k)}{ikc}\right], \tag{21a}$$

$$B(k)=\frac{1}{2}\left[\hat{a}(k)-\frac{\hat{b}(k)}{ikc}\right], \tag{21b}$$

which gives us the solution for $\hat{q}(k,t)$ in terms of the initial conditions

$$\hat{q}(k,t)=\frac{1}{2}\left[\hat{a}(k)+\frac{\hat{b}(k)}{ikc}\right]e^{ikct}+\frac{1}{2}\left[\hat{a}(k)-\frac{\hat{b}(k)}{ikc}\right]e^{-ikct} \tag{22}$$

We are essentially done. We have now expressed the FT of $q(x,t)$ in terms of the FT's of the initial conditions for the problem. The solution $q(x,t)$ is just the inverse FT of Eq. (22) [see Eq. (15b)],

$$q(x,t)=\frac{1}{\sqrt{2\pi}}\frac{1}{2}\int_{-\infty}^{\infty}\left\{\left[\hat{a}(k)+\frac{\hat{b}(k)}{ikc}\right]e^{ik(x+ct)}+\left[\hat{a}(k)-\frac{\hat{b}(k)}{ikc}\right]e^{ik(x-ct)}\right\}dk\,. \tag{23}$$

This is the initial-value-problem solution.[4] We can make it look exactly like Eq. (14) with a little bit more manipulation. To see this let's first rewrite Eq. (23) as

[4] Notice that $q(x,t)$ as expressed in Eq. (23) is the sum of two functions, $f(x+ct)$ and $g(x-ct)$!

$$q(x,t)=\frac{1}{\sqrt{2\pi}}\frac{1}{2}\int_{-\infty}^{\infty}\left\{\left[\hat{a}(k)e^{ik(x+ct)}+\hat{a}(k)e^{ik(x-ct)}\right]+\frac{1}{c}\left[\frac{\hat{b}(k)}{ik}\left(e^{ik(x+ct)}-e^{ik(x-ct)}\right)\right]\right\}dk\,. \tag{24}$$

The first two terms we recognize as $(1/2)[a(x+ct)+a(x-ct)]$, while we can use Eq. (5) to recognize the second half of the rhs of Eq. (24) as $(1/2c)\int_{x-ct}^{x+ct}b(x')dx'$. Thus Eq. (24) can be re-expressed as

$$q(x,t)=\frac{1}{2}\left[a(x+ct)+a(x-ct)+\frac{1}{c}\int_{x-ct}^{x+ct}b(x')dx'\right], \tag{25}$$

which is identical to Eq. (14).

Exercises

*__17.1 FT Properties__. If the FT of $f(x)$ is $h(k)$,
(**a**) show that the FT of $\left[e^{ik_0x}f(x)\right]$ is $h(k-k_0)$;
(**b**) show that the FT of $[x\,f(x)]$ is $ih'(k)$;
(**c**) show that the FT of $\left[x^2f(x)\right]$ is $-h''(k)$.

*__17.2__ Show that $(f*g)(x)=(g*f)(x)$ by
(**a**) directly by manipulating Eq. (7), the definition of convolution;
(**b**) by using Eq. (11), the result for the FT of $(f*g)(x)$.

*__17.3 Convolution and the Gaussian__. The function that has the same form as its Fourier transform is the Gaussian. Specifically if $f(x)=e^{-x^2/\sigma^2}$, its FT is given by $h(k)=\frac{\sigma}{\sqrt{2}}e^{-k^2(\sigma^2/4)}$. Using this fact, show that the convolution $(f_1*f_2)(x)$ of two Gaussian functions $f_1(x)=e^{-x^2/\sigma_1^2}$ and $f_2(x)=e^{-x^2/\sigma_2^2}$ is proportional to the Gaussian function $e^{-x^2/(\sigma_1^2+\sigma_2^2)}$. [Hint: you need not calculate any integrals to do this problem.]

17.4 The Rectangular Pulse.

Here you will explore the convolution theorem as it applies to a rectangular pulse and its convolution, a triangular pulse. We start with the function $f(x)$, a rectangular pulse of height H and width $2L$ centered at $x=0$. Elsewhere the function is zero.

(**a**) Graph $f(x)$

(**b**) Calculate Find $\hat{f}(k)$, the FT of $f(x)$. (This is a real function; express it as such.)

(**c**) Graph $\hat{f}(k)$.

(**d**) The function $(f*f)(x)$, the convolution of $f(x)$ with itself, is a triangle function of height $2LH^2$ and base $4L$ centered at zero. It is zero elsewhere. Graph this function.

(**e**) Write down the mathematical expression for $(f*f)(x)$ [that you graphed in (d)]. Then *directly* calculate $\left(f\hat{*}f\right)(k)$ using your functional form for $(f*f)(x)$. (Do not set H and L to specific values. Again, this is a real function; express it as such.)

(**f**) Graph your calculated transform $\left(f\hat{*}f\right)(k)$.

(**g**) Lastly, use $\hat{f}(k)$ and the convolution theorem to find $\left(f\hat{*}f\right)(k)$. Show that this is equal to the result in part (e).

17.5 FT Solution to the 1D Wave Equation. Eq. (23),

$$q(x,t)=\frac{1}{\sqrt{2\pi}}\frac{1}{2}\int_{-\infty}^{\infty}\left\{\left[\hat{a}(k)+\frac{\hat{b}(k)}{ikc}\right]e^{ik(x+ct)}+\left[\hat{a}(k)-\frac{\hat{b}(k)}{ikc}\right]e^{ik(x-ct)}\right\}dk\,, \tag{23}$$

is the formal solution to the initial-value problem.

(**a**) What kind of waves are described by the functions $\exp[ik(x+ct)]$ and $\exp[ik(x-ct)]$? Be as specific as possible!

(**b**) From a vector-space point of view, the functions $\exp[ik(x+ct)]$ and $\exp[ik(x-ct)]$ can be considered basis functions for the vector space that consists of solutions to the wave equation. Given this, what do the terms $\frac{1}{2}\left[\hat{a}(k)-\frac{i\hat{b}(k)}{kc}\right]$ and $\frac{1}{2}\left[\hat{a}(k)+\frac{i\hat{b}(k)}{kc}\right]$ represent?

(**c**) Given your answer in (b), how would you describe the solution $q(x,t)$ as written above? [Hint: the term *linear combination* should appear in your answer.]

(**d**) How are $\hat{a}(k)$ and $\hat{b}(k)$ related to the initial conditions $q(x,0)$ and $\frac{\partial q}{\partial t}(x,0)$? That is, write down expressions for $\hat{a}(k)$ and $\hat{b}(k)$ in terms of $q(x,0)$ and $\frac{\partial q}{\partial t}(x,0)$.

(**e**) Assume that the initial conditions $q(x,0)$ and $\frac{\partial q}{\partial t}(x,0)$ are real. Using your answer to (d), show that $\hat{a}(k) = \hat{a}^*(-k)$ and $\hat{b}(k) = \hat{b}^*(-k)$.

(**f**) Using the results from (e) you can now show that $q(x,t)$ is real if the initial conditions $q(x,0)$ and $\dot{q}(x,0)$ are both real, as follows. First, in Eq. (23) replace $\hat{a}(k)$ and $\hat{b}(k)$ by $\hat{a}^*(-k)$ and $\hat{b}^*(-k)$, respectively. Then make the change of variable $k \to -k$, $dk \to -dk$ in the integral (taking care with the limits of integration). Then compare Eq. (23) with your new expression for $q(x,t)$ and notice how they are related. From this comparison you should be able to conclude that $q(x,t)$ is real.

3D Wave Equation and Plane Waves / 3D Differential Operators

Overview and Motivation: We now extend the wave equation to three-dimensional space and look at some basic solutions to the 3D wave equation, which are known as plane waves. Although we will not discuss it, plane waves can be used as a basis for any solutions to the 3D wave equation, much as harmonic traveling waves can be used as a basis for solutions to the 1D wave equation. We then look at the gradient and Laplacian, which are linear differential operators that act on a scalar field. We also touch on the divergence, which operates on a vector field.

Key Mathematics: The 3D wave equation, plane waves, fields, and several 3D differential operators.

I. The 3D Wave Equation and Plane Waves

Before we introduce the 3D wave equation, let's think a bit about the 1D wave equation,

$$\frac{\partial^2 q}{\partial t^2} = c^2 \frac{\partial^2 q}{\partial x^2}. \tag{1}$$

Some of the simplest solutions to Eq. (1) are the harmonic, traveling-wave solutions

$$q_k^+(x,t) = A\, e^{i(kx-\omega t)}, \tag{2a}$$

$$q_k^-(x,t) = B\, e^{i(kx+\omega t)}, \tag{2b}$$

where, without loss of generality, we can assume that $\omega = |ck| > 0$.[1] Let's think about these solutions as a function of the wave vector k. First, we should remember that k is related to the wavelength via $k = 2\pi/\lambda$. Let's now specifically think about the solution $q_k^+(x,t)$. For this solution, if $k > 0$ then the wave propagates in the $+x$ direction, and if $k < 0$, then the wave propagates in the $-x$ direction. Thus, in either case, the wave propagates *in the direction of* k. Similarly, for the solution $q_k^-(x,t)$ the wave propagates in the direction opposite to the direction of k.

We now introduce the 3D wave equation and discuss solutions that are analogous to those in Eq. (2) for the 1D equation. The 3D extension of Eq. (1) can be obtained by adding two more spatial-derivative terms, yielding

[1] If we assume $\omega < 0$, then the two $\omega > 0$ solutions just map into each other.

$$\frac{\partial^2 q}{\partial t^2} = c^2\left(\frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} + \frac{\partial^2 q}{\partial z^2}\right) \tag{3}$$

where now $q = q(x,y,z,t)$ and x, y, and z are standard Cartesian coordinates. This equation can be used to describe, for example, the propagation of sound waves in a fluid. In that case q represents the longitudinal displacement of the fluid as the wave propagates through it.

The 3D solutions to Eq. (3) that are analogous to the 1D solutions expressed by Eq. (2) can be written as

$$q^{+}_{k_x,k_y,k_z}(x,y,z,t) = A\,e^{i\left(k_x x + k_y y + k_z z - \omega t\right)}, \tag{4a}$$

$$q^{-}_{k_x,k_y,k_z}(x,y,z,t) = B\,e^{i\left(k_x x + k_y y + k_z z + \omega t\right)} \tag{4b}$$

As you may suspect, the wave equation determines a relationship between the set $\{k_x, k_y, k_z\}$ and the frequency ω. Substituting either Eq. (4a) or (4b) into Eq. (3) yields

$$\omega^2 = c^2\left(k_x^2 + k_y^2 + k_z^2\right). \tag{5}$$

As above, we can assume $\omega > 0$, which gives

$$\omega = c\sqrt{k_x^2 + k_y^2 + k_z^2}\,,$$

the dispersion relation for the Eq. (4) solutions to the 3D wave equation.

The solutions in Eq. (4) can be also written in a more elegant form. If we define the 3D wave vector

$$\mathbf{k} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}} + k_z\hat{\mathbf{z}}, \tag{6}$$

and use the Cartesian-coordinate form of the position vector

$$\mathbf{r} = x\,\hat{\mathbf{x}} + y\,\hat{\mathbf{y}} + z\,\hat{\mathbf{z}}, \tag{7}$$

then we see that we can rewrite Eq. (4) as

$$q^{+}_{\mathbf{k}}(\mathbf{r},t) = A\,e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}, \tag{8a}$$

$$q_{\mathbf{k}}^{-}(\mathbf{r},t) = B\, e^{i(\mathbf{k}\cdot\mathbf{r}+\omega t)}, \tag{8b}$$

where $\mathbf{k}\cdot\mathbf{r} = k_x x + k_y y + k_z z$ is the standard dot product of two vectors. The dispersion relation can then also be written more compactly as

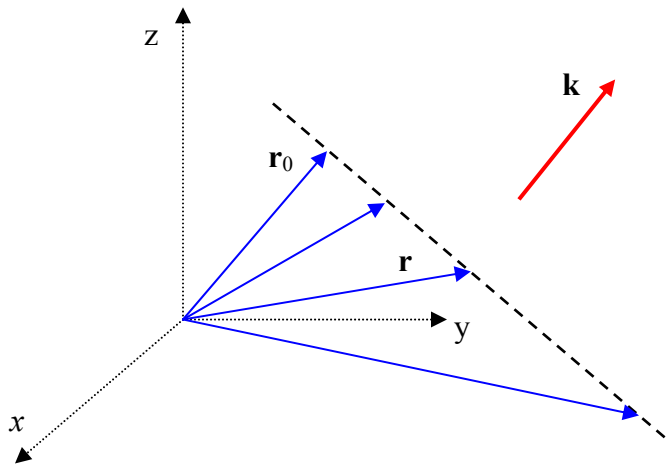
$$\omega = c\left|\mathbf{k}\right|. \tag{9}$$

It is also the case that the wavelength λ is related to $\mathbf{k}$ via $\left|\mathbf{k}\right| = 2\pi/\lambda$.

Analogous to the discussion about the direction of the 1D solutions, the wave in Eq. (8a) propagates in the $+\mathbf{k}$ direction while the wave in Eq. (8b) propagates in the $-\mathbf{k}$ direction. This is why one usually sees the form in Eq. (8a): the wave simply propagates in the direction that $\mathbf{k}$ points in this case.

These propagating solutions in Eq. (8) are known as **plane waves**. Why is that, you may ask? It is because at any given time the planes perpendicular to the propagation direction have the same value of the displacement of q.

Let's see that this is so. Consider the following picture.



Keep in mind that the wave vector $\mathbf{k}$ is a fixed quantity (for a given plane wave); its direction is indicated in the figure. The dotted line in the picture represents a plane

that is perpendicular to $\mathbf{k}$ and passes through the point in space defined by the vector $\mathbf{r}$. Now consider the dot product

$$\mathbf{k}\cdot\mathbf{r} = |\mathbf{k}|\cdot|\mathbf{r}|\cos(\theta) \tag{10}$$

This is simply equal to $|\mathbf{k}|\cdot|\mathbf{r}_0|$, where $\mathbf{r}_0$ is the position vector in the plane that is parallel to $\mathbf{k}$. Furthermore, for *any* position vector in the plane the dot product with $\mathbf{k}$ has this same value. That is, for any vector $\mathbf{r}$ in the plane $\mathbf{k}\cdot\mathbf{r}$ is constant. Thus, the plane-wave function $Ae^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ has the same value for all points $\mathbf{r}$ in the plane.

A simple example of a plane wave is one that is propagating in the z direction. In that case the q^+ plane wave is $q^+_{0,0,k_z}(z,t) = Ae^{i(k_z z-\omega t)}$. Notice that this wave does not depend upon x or y. That is, for a given value of z, the wave has the same displacement for all values of x and y. That is, it has the same displacement for any point on a plane with the same value of z.

II. Some 3D Linear Differential Operators

A. The Laplacian

The combination of spatial derivatives on the rhs of Eq. (3),

$$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}, \tag{11}$$

is the Cartesian-coordinate version of the linear differential operator know as the **Laplacian**, generically designated as either Δ or ∇^2 (**del squared**). The del-squared representation is often used because the Laplacian can be though of as two successive (although different) applications of the differential expression that is simply known as **del** , which is represented by the symbol ∇.[2]

In Cartesian coordinates

$$\nabla = \frac{\partial}{\partial x}\hat{\mathbf{x}}+\frac{\partial}{\partial y}\hat{\mathbf{y}}+\frac{\partial}{\partial x}\hat{\mathbf{z}}\,. \tag{12}$$

The Laplacian ∇^2 can thus be written in Cartesian coordinates as

[2] As we shall see below, ∇ can be used in the representation of several operators. It is thus probably best not to think of ∇ itself as an operator.

$$\nabla\cdot\nabla=\left(\frac{\partial}{\partial x}\hat{\mathbf{x}}+\frac{\partial}{\partial y}\hat{\mathbf{y}}+\frac{\partial}{\partial x}\hat{\mathbf{z}}\right)\cdot\left(\frac{\partial}{\partial x}\hat{\mathbf{x}}+\frac{\partial}{\partial y}\hat{\mathbf{y}}+\frac{\partial}{\partial x}\hat{\mathbf{z}}\right). \tag{13}$$

We now consider the application of ∇^2 to a function $f(x,y,z)$, but we do it "one del at a time." That is, writing $\nabla^2 f(x,y,z)$ as $\nabla\cdot[\nabla f(x,y,z)]$, we first consider the piece $\nabla f(x,y,z)$. Afterwards we look at $\nabla\cdot[\nabla f(x,y,z)]$, which we usually simply write as $\nabla\cdot\nabla f(x,y,z)$.

However, before we do this, let's make sure that we understand the concept of a field. A **field** is simply a mathematical quantity that has a value assigned to each point in space. The function $f(x,y,z)$ is known as a **scalar field**, because $f(x,y,z)$ assigns a scalar to each point in space. A **vector field** is a function that assigns a vector to each point in space. An electric field is an example of a vector field.

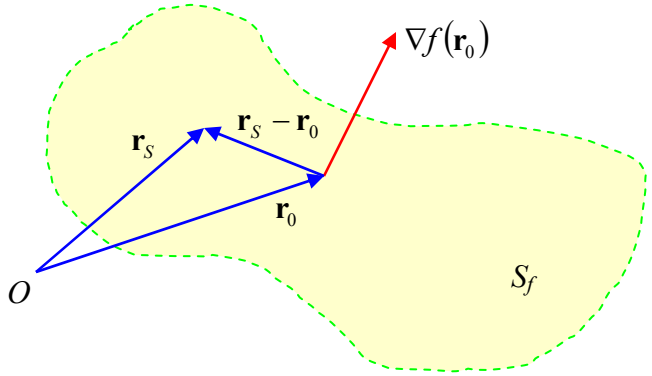
B. The Gradient

The quantity ∇f is know as the **gradient** of f. Let's take a closer look at ∇f. Applying Eq. (12) (the Cartesian-coordinate version of ∇) to $f(x,y,z)$ produces

$$\nabla f(x,y,z)=\frac{\partial f}{\partial x}\hat{\mathbf{x}}+\frac{\partial f}{\partial y}\hat{\mathbf{y}}+\frac{\partial f}{\partial z}\hat{\mathbf{z}}. \tag{14}$$

Although not explicitly shown, each term on the rhs is a function of x, y, and z. Thus ∇f is a vector field because it assigns a vector to each point in space. Simply put, the gradient of a scalar field is a vector field.

An important property of $\nabla f(\mathbf{r})$ is that $\nabla f(\mathbf{r})$ is perpendicular to the surface of constant f that contains $\mathbf{r}$ (where $\mathbf{r}$ is any position vector). Let's use a bit of vector calculus to show this. Consider the picture below. The surface S_f is the surface of constant f that contains (the end of) $\mathbf{r}_0$. The vector $\mathbf{r}_S$ is also assumed to lie on this surface. So we wish to show that $\nabla f(\mathbf{r}_0)$ is perpendicular to S_f at $\mathbf{r}_0$.



We now assume that $\mathbf{r}_S$ is close enough to $\mathbf{r}_0$ that we can write the function $f(\mathbf{r}_S) = f(x_S, y_S, z_S)$ as a Taylor series expanded about the point $\mathbf{r}_0 = (x_0, y_0, z_0)$,

$$f(x_S, y_S, z_S) = f(x_0, y_0, z_0) + \left.\frac{\partial f}{\partial x}\right|_{\mathbf{r}_0} (x_S - x_0) + \left.\frac{\partial f}{\partial y}\right|_{\mathbf{r}_0} (y_S - y_0) + \left.\frac{\partial f}{\partial z}\right|_{\mathbf{r}_0} (z_S - z_0) + \ldots \tag{15}$$

Now this equation can be expressed in coordinate-independent form as

$$f(\mathbf{r}_S) = f(\mathbf{r}_0) + \nabla f(\mathbf{r}_0) \cdot (\mathbf{r}_S - \mathbf{r}_0) + \ldots \tag{16}$$

If we now assume that $\mathbf{r}_S$ is close enough to $\mathbf{r}_0$ so that the curvature of the surface is negligible, then the higher-order terms can be neglected. Then, because $f(\mathbf{r}_S) = f(\mathbf{r}_0)$ (both vectors are on the surface S_f), we have

$$\nabla f(\mathbf{r}_0) \cdot (\mathbf{r}_S - \mathbf{r}_0) = 0 . \tag{17}$$

And because $(\mathbf{r}_S - \mathbf{r}_0)$ lies in the surface[3] we have the result that $\nabla f(\mathbf{r}_0)$ is perpendicular to the surface S_f at the point $\mathbf{r}_0$. *QED.*

A concept closely associated with the gradient is the **directional derivative**. If we have some unit position vector $\hat{\mathbf{r}}_d$, then the directional derivative of $f(\mathbf{r})$ in the direction of $\hat{\mathbf{r}}_d$ is defined as

$$\nabla f(\mathbf{r}) \cdot \hat{\mathbf{r}}_d \tag{18}$$

[3] The surface is essentially planar in the vicinity of $\mathbf{r}_S$ and $\mathbf{r}_0$ because of the proximity of $\mathbf{r}_S$ to $\mathbf{r}_0$.

Physically, the directional derivative tells you how fast the function $f(\mathbf{r})$ changes in the direction of $\hat{\mathbf{r}}_d$. What kind of field is this quantity? Notice that you can also think of the directional derivative as the scalar component of $\nabla f(\mathbf{r})$ in the $\hat{\mathbf{r}}_d$ direction.

A straightforward application of the gradient is found in classical mechanics. If $U(x,y,z)$ is a potential-energy function associated with a particle, then the force on the particle associated with that potential energy is given by $\mathbf{F}(x,y,z) = -\nabla U(x,y,z)$, which is a vector field (a force field!).

As an example, let's consider the gravitational force on a particle near the Earth's surface. If we define our coordinate system such that z points upwards and x and y lie in a horizontal plane, then the gravitational potential energy of a particle with mass m is given by $U(x,y,z) = mg(z - z_0)$, where z_0 is an arbitrary constant and $g \approx 9.8$ m/s^2. The force on the particle is then given by $-\nabla U(x,y,z) = -mg\hat{\mathbf{z}}$. What are surfaces of constant $U(x,y,z)$ in this case? These are simply horizontal planes (each one at a constant value of z). Notice that these planes are indeed perpendicular to the force field $-mg\hat{\mathbf{z}}$, which points downward at all points in space.

C. Divergence

Now that we have some feel for the meaning of $\nabla f(\mathbf{r})$, let's now apply the second del to $\nabla f(\mathbf{r})$, which gives us $\nabla \cdot \nabla f(\mathbf{r}) = \nabla^2 f(\mathbf{r})$. But before we do this, maybe we should first say a few words about $\nabla \cdot$ operating on any vector field $\mathbf{V}(\mathbf{r})$. Writing $\mathbf{V}(\mathbf{r})$ as $V_x\hat{\mathbf{x}} + V_y\hat{\mathbf{y}} + V_z\hat{\mathbf{z}}$ and using the Cartesian-coordinate form of $\nabla \cdot$, we have

$$\begin{aligned} \nabla \cdot \mathbf{V}(\mathbf{r}) &= \left(\frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial x}\hat{\mathbf{z}} \right) \cdot \left(V_x\hat{\mathbf{x}} + V_y\hat{\mathbf{y}} + V_z\hat{\mathbf{z}} \right) \\ &= \frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial x} \end{aligned} . \tag{19}$$

The quantity $\nabla \cdot \mathbf{V}(\mathbf{r})$ is called the **divergence** of the vector field $\mathbf{V}(\mathbf{r})$. So what kind of object is $\nabla \cdot \mathbf{V}(\mathbf{r})$? Because it assigns a scalar to each point in space it is a scalar field.[4] Thus we see that the gradient of a scalar field is a vector field, while the divergence of a vector field is a scalar field.

If we now let $\mathbf{V}(\mathbf{r})$ equal $\nabla f(\mathbf{r})$, we then get [using Eq. (14)]

[4] We will discuss the divergence in more detail in a later lecture. Stay tuned!

$$\nabla\cdot\nabla f(\mathbf{r}) = \left(\frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial x}\hat{\mathbf{z}}\right)\cdot\frac{\partial f}{\partial x}\hat{\mathbf{x}} + \frac{\partial f}{\partial y}\hat{\mathbf{y}} + \frac{\partial f}{\partial x}\hat{\mathbf{z}} \\ = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \quad . \tag{20}$$

So we see that the Laplacian of f, $\nabla^2 f$, is the divergence of the gradient of f. Thus, $\nabla^2 f$ is a scalar field.

III. Some Final Remarks

Using the generic form of the Laplacian, Eq. (3) can be written in coordinate-independent form as

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \nabla^2 q\,. \tag{21}$$

In the next lecture we will look at some more solutions to Eq. (21) using Eq. (3), the Cartesian-coordinate representation, but after that we will look at solutions to Eq. (21) using some different coordinate systems – cylindrical and spherical-polar. The representation of Equation (21) in each coordinate system will look vastly different. Nonetheless, in each case we will be solving a version of Eq. (21), the 3D wave equation.

Exercises

***18.1 Plane Waves**. Consider the solution $q^+_{\mathbf{k}}(\mathbf{r},t) = A\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ to the 3D wave equation. Assume that $\omega > 0$.
(**a**) Calculate $\nabla q^+_{\mathbf{k}}(\mathbf{r},t)$. In what direction does $\nabla q^+_{\mathbf{k}}(\mathbf{r},t)$ point? Thus describe constant surfaces of $q^+_{\mathbf{k}}(\mathbf{r},t)$ (for some fixed value of t).
(**b**) In what direction does $q^+_{\mathbf{k}}(\mathbf{r},t) = A\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ move? What is the wavelength λ of this wave? What is the dispersion relation $\omega(\mathbf{k})$ for this wave?
(**c**) Show that the sum of $q^+_{\mathbf{k}}(\mathbf{r},t) = A\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ and $q^-_{\mathbf{k}}(\mathbf{r},t) = B\,e^{i(\mathbf{k}\cdot\mathbf{r}+\omega t)}$ is a standing wave if $B = A$. (Make sure that you write down the specific form of this standing wave.) What property of the wave equation allows you to combine solutions to produce another solution?

*__18.2 Divergence and Gradient__. Consider the function $f(x,y,z)=\frac{1}{x^2}+\frac{2}{y^2}+\frac{3}{z^2}$.

(**a**) Is it appropriate to calculate the divergence or gradient of this function? Calculate whichever is appropriate.
(**b**) You should now have a new function that you calculated in part (**a**). What kind of function is it? Calculate either the gradient or divergence of this new function, whichever is appropriate.

*__18.3 Divergence__. Using the Cartesian-coordinate form of the divergence, $\nabla\cdot=\left(\frac{\partial}{\partial x}\hat{\mathbf{x}}+\frac{\partial}{\partial y}\hat{\mathbf{y}}+\frac{\partial}{\partial x}\hat{\mathbf{z}}\right)\cdot$, compute the following.

(**a**) $\mathbf{E}(\mathbf{r})=\frac{\mathbf{r}}{r^3}$, where $r=\sqrt{x^2+y^2+z^2}>0$. (Coulomb electric field)

(**b**) $\mathbf{B}(\mathbf{r})=-\frac{y}{x^2+y^2}\hat{\mathbf{x}}+\frac{x}{x^2+y^2}\hat{\mathbf{y}}$, $x^2+y^2>0$. (magnetic field outside a long wire)

*__18.4__ Let f and g be two scalar fields. Using the Cartesian-coordinate form of del, show that $\nabla\cdot(f\nabla g)=\nabla f\cdot\nabla g+f\nabla^2 g$. What kind of field is $\nabla\cdot(f\nabla g)$?

*__18.5__ Using (a) Cartesian coordinates, and then (b) spherical-polar coordinates, calculate the divergence of $\mathbf{E}(\mathbf{r})=\mathbf{r}$ (electric field inside a uniform ball of charge). For a field $V(\mathbf{r})$that only depends upon the coordinate r, the divergence in spherical-polar coordinates is given by $\nabla\cdot\mathbf{F}(\mathbf{r})=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2F_r\right)$.

Separation of Variables in Cartesian Coordinates

Overview and Motivation: Today we begin a more in-depth look at the 3D wave equation. We introduce a technique for finding solutions to partial differential equations that is known as separation of variables. We first do this for the wave equation written in Cartesian coordinates. In subsequent lectures we will do the same using cylindrical and spherical-polar coordinates. The technique is applicable not only to the wave equation, but to a wide variety of partial differential equations that are important in physics.

Key Mathematics: The technique of separation of variables!

I. Separable Solutions

Last time we introduced the 3D wave equation, which can be written in Cartesian coordinates as

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \frac{\partial^2 q}{\partial x^2} + \frac{\partial^2 q}{\partial y^2} + \frac{\partial^2 q}{\partial z^2}, \tag{1}$$

and we spent some time looking at the plane-wave solutions

$$q^{+}_{k_x,k_y,k_z}(x,y,z,t) = A^{+}e^{i\left(k_x x + k_y y + k_z z - \omega t\right)}, \tag{2a}$$

$$q^{-}_{k_x,k_y,k_z}(x,y,z,t) = A^{-}e^{i\left(k_x x + k_y y + k_z z + \omega t\right)}, \tag{2b}$$

where $\omega = c|\mathbf{k}|$ is the familiar dispersion relation. Equation (2a) describes a wave that travels in the $\mathbf{k} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}} + k_z\hat{\mathbf{z}}$ direction with wavelength $\lambda = 2\pi/|\mathbf{k}|$, while Eq. (2b) describes a similar wave that travels in the $-\mathbf{k}$ direction.

Today we introduce **separation of variables**, a technique that leads to **separable** (also known as **product**) solutions. A separable solution is of the form

$$q(x,y,z,t) = X(x)Y(y)Z(z)T(t). \tag{3}$$

That is, the function $q(x,y,z,t)$ is a product of the functions $X(x)$, $Y(y)$, $Z(z)$, and $T(t)$.

So how do we find these solutions? Well, let's just substitute the rhs of Eq. (3) into Eq. (1) and see what happens. With this substitution Eq. (1) becomes

$$\frac{1}{c^2} X\,Y\,Z\,T'' = X''YZT + XY''ZT + XYZ''T\,, \tag{4}$$

where we have suppressed the independent variables and the double prime indicates the second derivative of the function with respect to its argument. Note that because each of these functions is a function of only one variable, all derivatives are now ordinary derivatives. Equation (4) looks kind of ugly, but notice what happens if we divide Eq. (4) by $q(x,y,z,t) = X(x)Y(y)Z(z)T(t)$. We then get

$$\frac{1}{c^2}\frac{T''}{T} = \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}. \tag{5}$$

Now here is where the magic happens. Notice that each term is only a function of its associated independent variable. So for example, if we vary t only the term on the lhs of Eq. (5) can vary. But, because none of the other terms depends upon t, the rhs cannot vary, which means that the lhs cannot vary, which means that T''/T is *independent* of t! Following the same logic for each of the other terms means that each term is constant. So we can write

$$\frac{1}{c^2}\frac{T''}{T} = \alpha\,, \qquad \frac{X''}{X} = \beta\,, \qquad \frac{Y''}{Y} = \gamma\,, \qquad \frac{Z''}{Z} = \delta \tag{6a) – (6d}$$

where the constants α, β, γ, and δ are known as **separation constants**. However, only three of them are independent because Equation (5) tells us that

$$\alpha = \beta + \gamma + \delta\,. \tag{7}$$

Notice, by demanding a product solution the partial differential wave equation has transformed into four ordinary differential equations. We can easily solve all of these equations. Let's start with the equation for $T(t)$,

$$T''(t) - \alpha c^2 T(t) = 0\,. \tag{8}$$

This is essentially the harmonic oscillator equation (if α is real and <0), and so it has the two, linearly independent solutions

$$T(t) = T_0 e^{\pm c\sqrt{\alpha}\,t}\,, \tag{9a}$$

where T_0 is some undetermined constant. Similarly, the X, Y, and Z equations have solutions

$$X(t) = X_0 e^{\pm\sqrt{\beta}\,x}, \tag{9b}$$

$$Y(t) = Y_0 e^{\pm\sqrt{\gamma}\,y}, \tag{9c}$$

$$Z(t) = Z_0 e^{\pm\sqrt{\delta}\,z}, \tag{9d}$$

Putting this all together gives us a solution of the form

$$q(x,y,z,t) = X_0\,Y_0\,Z_0\,T_0\;e^{\pm\sqrt{\beta}\,x}\,e^{\pm\sqrt{\gamma}\,y}\,e^{\pm\sqrt{\delta}\,z}\,e^{\pm c\sqrt{\alpha}\,t}. \tag{10}$$

II. Some Physics Added In

Notice that the solution in Eq. (10) can have all sorts of behavior. For example, if the constant β is real and positive, then the x dependent part of the solution can either exponentially increase or decrease with increasing x (depending upon the sign in the exponent). This points out the fact that separation-of-variables solutions often give you more than you really need in any given situation. For example, if we are looking for solutions to the wave equation that are physically meaningful as $x \to \infty$, we are (probably) not going to be interested in a solution that exponentially increases with increasing x.

With that in mind, let's see what the constraints on the separation constants must be if we are only interested in purely oscillatory solutions (in all independent variables). Let's consider the x dependent part of the solution. If $e^{\pm\sqrt{\beta}\,x}$ is to only oscillate then it must be of the form $e^{\pm ik_x x}$, where k_x is real. Then, if we write a generally complex β as $\beta = \beta_1 + i\beta_2$ we have $\sqrt{\beta_1 + i\beta_2} = ik_x$ which implies $\beta_1 + i\beta_2 = -k_x^2$. Thus $\beta_2 = 0$ and $\beta_1 = -k_x^2$. That is, β is real and negative. Similarly, γ and δ must be real and negative. Eq. (7) then implies that α is also real and negative. So if we rename the constants as

$$\beta = -k_x^2, \qquad \gamma = -k_y^2, \qquad \delta = -k_z^2, \qquad \alpha = -\omega^2/c^2, \tag{11a) – (11d}$$

(where k_x, k_y, k_z, and ω are all real) then Eq. (10) can be rewritten as

$$q(x,y,z,t) = A\,e^{\pm ik_x x}\,e^{\pm ik_y y}\,e^{\pm ik_z z}\,e^{\pm i\omega t} \tag{12}$$

where $A = X_0\,Y_0\,Z_0\,T_0$ is an arbitrary constant. Eq. (7) can now be written as $\omega^2/c^2 = k_x^2 + k_y^2 + k_z^2$, which is the well known dispersion relation! Now k_x, k_y, and k_z

can be positive or negative, so we don't need the ± on the spatial-function exponents, and so we are left with two linearly independent solutions

$$q^{+}_{k_x,k_y,k_z}(x,y,z,t) = A^{+}e^{i(k_x x+k_y y+k_z z-\omega t)}, \tag{13a}$$

$$q^{-}_{k_x,k_y,k_z}(x,y,z,t) = A^{-}e^{i(k_x x+k_y y+k_z z+\omega t)}, \tag{13b}$$

which are the plane-wave solutions of Eq. (2)! So, by demanding that the separable solutions to the wave equation oscillate, we have ended up with the plane-wave solutions that we discussed in the last lecture.

III. Utility of the Separable Solutions

Because they are product solutions, the separable solutions are pretty specialized. That is, there are many solutions to the wave equation that *cannot* be written as a product solution. And so you may ask, what is the usefulness of these solutions? There are two parts to the answer. The first is that sometimes these solutions have intrinsic interest. For example, in the case of the time-dependent Schrödinger equation the separable solutions (with some appropriate physics thrown in) are the energy eigenstates of the system. The second, and perhaps more important, part of the answer is that a basis can be constructed from the set of separable solutions that can be used to represent any solution.

Let's think about this statement with regards to the wave equation. Let's first consider the 1D wave equation. Back in the Lecture 17 notes we solved the initial-value problem on the interval $-\infty < x < \infty$. The solution to that problem can be written as

$$q(x,t) = \frac{1}{\sqrt{2\pi}}\frac{1}{2}\int_{-\infty}^{\infty} dk \left\{ \left[\hat{a}(k) + \frac{\hat{b}(k)}{i|k|c} \right] e^{i(kx+\omega t)} + \left[\hat{a}(k) - \frac{\hat{b}(k)}{i|k|c} \right] e^{i(kx-\omega t)} \right\}, \tag{14}$$

where $\hat{a}(k)$ and $\hat{b}(k)$ are the Fourier transforms of the initial conditions, and $\omega = c|k|$ is the dispersion relation. Notice that in Eq. (14) we have written the general solution $q(x,t)$ as a linear combination of the functions $e^{i(kx+\omega t)}$ and $e^{i(kx-\omega t)}$. Although we did not go through the separation of variables procedure for the 1D wave equation to produce these solutions, by writing these functions as $e^{ikx}e^{i\omega t}$ and $e^{ikx}e^{-i\omega t}$, we readily see that they are indeed product solutions.

Similarly, for the 3D wave equation we can write the solution to the initial value problem as a linear combination of the separable (plane-wave) solutions [Eq. (13)]

$$q(\mathbf{r},t)=\frac{1}{(2\pi)^{3/2}}\frac{1}{2}\int d^3k\left\{\left[\hat{a}(\mathbf{k})+\frac{\hat{b}(\mathbf{k})}{i|\mathbf{k}|c}\right]e^{i(\mathbf{k}\cdot\mathbf{r}+\omega t)}+\left[\hat{a}(\mathbf{k})-\frac{\hat{b}(\mathbf{k})}{i|\mathbf{k}|c}\right]e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\right\}, \tag{15}$$

where $\mathbf{k}\cdot\mathbf{r}=k_x x+k_y y+k_z z$, $\int d^3k=\int_{-\infty}^{\infty}dk_x\int_{-\infty}^{\infty}dk_y\int_{-\infty}^{\infty}dk_z$, $\omega=c\sqrt{k_x^2+k_y^2+k_z^2}$, and $\hat{a}(\mathbf{k})$ and $\hat{b}(\mathbf{k})$ are the 3D Fourier transforms of the initial conditions.

In the coming lectures we will look at separable solutions in cylindrical and spherical-polar coordinates. While we will not do a lot with the general solution written as a linear combination of these solutions, we should keep in mind that, in principle, it can be done.

Exercises

19.1 Heat Equation. A partial differential equation known as the heat equation, which is used to describe heat or temperature flow in an object, is given by $\nabla^2 q=\frac{1}{\lambda}\frac{\partial q}{\partial t}$, where $\lambda>0$.

(**a**) If there is no y or z dependence to the problem, write down a simplified version of this equation.

(**b**) Use separation of variables to find two ordinary differential equations, one in x and one in t. What are the orders of these two equations? Are they linear or nonlinear?

(**c**) Find the general solutions to the two ordinary differential equations. Thus write down the general separable solutions to the heat equation. [Note: there should be *two* linearly independent solutions.]

(**d**) In solving the heat equation, you should have found that $X''(x)/X(x)=C$, where C is some constant. Assume that this constant is real. If $C>0$, describe the behavior of the solutions vs x and t. In what ways are these solutions like solutions to the wave equation? In what ways are they different?

(**e**) If $C<0$, describe the behavior of the solutions vs x and t. In what ways are these solutions like solutions to the wave equation? In what ways are they different?

19.2 **Normal Modes Inside a Rectangular Room: Here we consider sound waves inside a rectangular room with one corner located at the origin and occupying space as indicated: $0 < x < L_x$, $0 < y < L_y$, $0 < z < L_z$. While we could deal with displacement (a vector field), it is easier to think about the pressure which is also governed by the wave equation, but is a scalar field. The boundary conditions on the pressure $p(x,y,z,t)$ are $\frac{\partial p}{\partial x} = 0$ at $x = 0$ and $x = L_x$, $\frac{\partial p}{\partial y} = 0$ at $y = 0$ and $y = L_y$, and $\frac{\partial p}{\partial z} = 0$ at $z = 0$ and $z = L_z$.

(**a**) As discussed in the notes, the separable *traveling-wave* solutions to the wave equation can be written (with q replaced by p) as $p^{\pm}_{k_x,k_y,k_z}(x,y,z,t) = A^{\pm} e^{i(k_x x + k_y y + k_z z \mp \omega t)}$ where $\omega = c\sqrt{k_x^2 + k_y^2 + k_z^2}$. However, we could have expressed the separable solutions as the *standing-wave* solutions

$$p^{\pm}_{k_x k_y k_z}(x,y,z,t) = \left[A_x \sin(k_x x) + B_x \cos(k_x x)\right]\left[A_y \sin(k_y y) + B_y \cos(k_y y)\right] \times \left[A_z \sin(k_z z) + B_z \cos(k_z z)\right] e^{\pm i\omega t}$$

Starting with this standing-wave form, find the specific solutions that satisfy the above boundary conditions. Note, these solutions should be labeled with three integers; call these integers n_x, n_y, and n_z. Express the allowed frequencies ω as a function of n_x, n_y, and n_z, the wave velocity c, and the dimensions of the room.

(**b**) The solutions that you found in (a) describe the *normal modes* for sound waves in a typical room where L_x and L_y are the widths and L_z is the height of the room. Consider a room of dimensions 10 ft × 11 ft × 8 ft. Calculate the frequencies ($f(n_x,n_y,n_z) = \omega(n_x,n_y,n_z)/2\pi$) of the 10 lowest-frequency room modes, and order them from lowest to highest frequency. For the speed of sound you may use 330 m/s.

(**c**) These lowest-frequency modes often wreak havoc with sound reproduction because they serve to amplify, through resonance, reproduced frequencies near their (resonance) frequencies. This is especially troublesome if two (or more) modes have frequencies that are close together (degenerate). For example a 10' × 10' × 10' room would have its three lowest modes at exactly the same frequency. Are any of the modes you calculated in (b) degenerate or nearly so?

The Wave Equation in Cylindrical Coordinates

Overview and Motivation: While Cartesian coordinates are attractive because of their simplicity, there are many problems whose symmetry makes it easier to use a different system of coordinates. For example, there are times when a problem has cylindrical symmetry (the fields produced by an infinitely long, straight wire, for example). In this case it is easier to use cylindrical coordinates. So today we begin our discussion of the wave equation in cylindrical coordinates.

Key Mathematics: Cylindrical coordinates and the chain rule for calculating derivatives.

I. Transforming the Wave Equation

As previously mentioned the (spatial) coordinate independent wave equation

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \nabla^2 q \tag{1}$$

can take on different forms, depending upon the coordinate system in use. In Cartesian coordinates the Laplacian ∇^2 is expressed as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

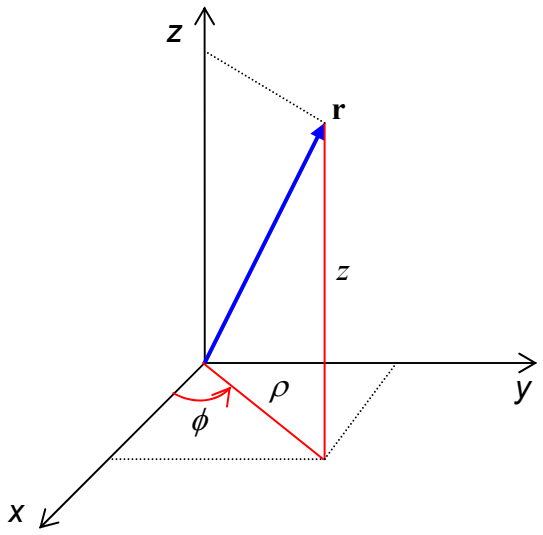
Our first goal is to re-express ∇^2 in terms of cylindrical coordinates (ρ, ϕ, z), which are defined in terms of the Cartesian coordinates (x, y, z) as

$$\rho = \left(x^2 + y^2\right)^{1/2}, \tag{2a}$$

$$\phi = \arctan\left(\frac{y}{x}\right), \tag{2b}$$

$$z = z. \tag{2c}$$

The following picture illustrates the relationships expressed by Eq. (2). For the point given by the vector $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$, the coordinate ρ is the distance of that point from the z axis, the coordinate ϕ is the angle of the projection of the vector onto the x-y plane from the x axis toward the y axis, and z is the (signed) distance of the point from the x-y plane. Note that $\rho \geq 0$ and we can restrict $0 \leq \phi < 2\pi$.



In order to express ∇^2 in terms of these new coordinates we start with a function $f(\rho,\phi,z)$ and consider it to be function of x, y, and z *through* the variables ρ, ϕ, and z by writing

$$f = f[\rho(x,y,z),\phi(x,y,z),z(x,y,z)]. \tag{3}$$

Then, for example, using the chain rule we can write

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial x} \tag{4}$$

Notice that this equation (as well as some later equations) have two types of terms. The first type is a derivative of the function f, while the second type is a derivative of a new coordinate with respect to an old coordinate. The goal here is to use the relationship between the two coordinate systems [Eq. (2)] to write the second type of term as a function of the new set of coordinates ρ, ϕ, and z. Then equations such as Eq. (4) will be entirely expressed in terms of the new coordinate system.

For the particular case at hand the transformation is a bit simpler than the general case because [see Eq. (2)] $\rho = \rho(x,y)$, $\phi = \phi(x,y)$, and $z = z(z)$. Thus Eq. (3) simplifies to

$$f = f[\rho(x,y),\phi(x,y),z(z)], \tag{5}$$

so that Eq. (4) reduces to

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}. \tag{6}$$

Let's now express the first term, $\partial^2 f/\partial x^2$, as a function of cylindrical coordinates. We do this by calculating another derivative of Eq. (6) with respect to x.

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial \rho}\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}\right). \tag{7}$$

Now we must be a bit careful here. We must use the chain rule on the functions $\partial f/\partial \rho$ and $\partial f/\partial \phi$ because they are functions of ρ and ϕ [as is f, see Eq. (5)]. However, we do not need to use the chain rule on the terms $\partial \rho/\partial x$ and $\partial \phi/\partial x$ because they are both functions of x and y [as are ρ and ϕ, see. Eq. (2)]. With this in mind Eq. (7) becomes

$$\frac{\partial^2 f}{\partial x^2} = \left(\frac{\partial^2 f}{\partial \rho^2}\frac{\partial \rho}{\partial x} + \frac{\partial^2 f}{\partial \phi \partial \rho}\frac{\partial \phi}{\partial x}\right)\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \rho}\frac{\partial^2 \rho}{\partial x^2} + \left(\frac{\partial^2 f}{\partial \rho \partial \phi}\frac{\partial \rho}{\partial x} + \frac{\partial^2 f}{\partial \phi^2}\frac{\partial \phi}{\partial x}\right)\frac{\partial \phi}{\partial x} + \frac{\partial f}{\partial \phi}\frac{\partial^2 \phi}{\partial x^2}, \tag{8}$$

which expands to

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial \rho^2}\left(\frac{\partial \rho}{\partial x}\right)^2 + \frac{\partial^2 f}{\partial \phi \partial \rho}\frac{\partial \phi}{\partial x}\frac{\partial \rho}{\partial x} + \frac{\partial f}{\partial \rho}\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 f}{\partial \rho \partial \phi}\frac{\partial \rho}{\partial x}\frac{\partial \phi}{\partial x} + \frac{\partial^2 f}{\partial \phi^2}\left(\frac{\partial \phi}{\partial x}\right)^2 + \frac{\partial f}{\partial \phi}\frac{\partial^2 \phi}{\partial x^2}. \tag{9}$$

You can see that this process is rather tedious! Now to eliminate the old variables x and y from Eq. (9) we must calculate the quantities

$$\frac{\partial \rho}{\partial x}, \qquad \frac{\partial \phi}{\partial x}, \qquad \frac{\partial^2 \rho}{\partial x^2}, \qquad \frac{\partial^2 \phi}{\partial x^2} \tag{10a) – (10d)}$$

and express them in terms of ρ and ϕ. Using Eq. (2a) we calculate the first of these terms as

$$\frac{\partial \rho}{\partial x} = \frac{\partial\left[\left(x^2 + y^2\right)^{1/2}\right]}{\partial x} = \frac{1}{2}\left(x^2 + y^2\right)^{-1/2} 2x = \frac{x}{\left(x^2 + y^2\right)^{1/2}}, \tag{11}$$

Now $x = \rho\cos(\phi)$ and $\rho^2 = x^2 + y^2$ so Eq. (11) becomes

$$\frac{\partial \rho}{\partial x} = \frac{\rho \cos(\phi)}{\rho} = \cos(\phi). \tag{12}$$

Similarly, using

$$\frac{\partial[\arctan(u)]}{\partial x} = \frac{1}{1+u^2}\frac{\partial u}{\partial x} \tag{13}$$

and Eq. (2b) we have

$$\frac{\partial \phi}{\partial x} = \frac{\partial[\arctan(y/x)]}{\partial x} = \frac{1}{1+(y/x)^2}\frac{-y}{x^2} = \frac{-y}{x^2+y^2}. \tag{14}$$

Using $y = \rho\sin(\phi)$ and $\rho^2 = x^2 + y^2$, we now re-express Eq. (14) in terms of the new coordinates as

$$\frac{\partial \phi}{\partial x} = \frac{-\rho\sin(\phi)}{\rho^2} = \frac{-\sin(\phi)}{\rho}. \tag{15}$$

In similar fashion one can express the second derivatives [Eq. (9c) and Eq. (9d)], in terms of ρ and ϕ as

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\sin^2(\phi)}{\rho} \tag{16}$$

and

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{2\cos(\phi)\sin(\phi)}{\rho^2}. \tag{17}$$

If we now insert Eqs. (12), (15), (16) and (17) into Eq. (9) we obtain

$$\begin{aligned}\frac{\partial^2 f}{\partial x^2} = {} & \frac{\partial^2 f}{\partial \rho^2}\cos^2(\phi) - \frac{\partial^2 f}{\partial \phi \partial \rho}\frac{\sin(\phi)\cos(\phi)}{\rho} + \frac{\partial f}{\partial \rho}\frac{\sin^2(\phi)}{\rho} \\ & - \frac{\partial^2 f}{\partial \rho \partial \phi}\frac{\sin(\phi)\cos(\phi)}{\rho} + \frac{\partial^2 f}{\partial \phi^2}\frac{\sin^2(\phi)}{\rho^2} + \frac{\partial f}{\partial \phi}\frac{2\cos(\phi)\sin(\phi)}{\rho^2}.\end{aligned} \tag{18}$$

So we have now expressed the first term of the Laplacian (acting on a function f) $\partial^2 f/\partial x^2$ in terms of cylindrical coordinates.

In a manner analogous to the procedure that we have just carried out one can also derive the result[1]

$$\begin{aligned}\frac{\partial^2 f}{\partial y^2} &= \frac{\partial^2 f}{\partial \rho^2}\sin^2(\phi) + \frac{\partial^2 f}{\partial \phi \partial \rho}\frac{\sin(\phi)\cos(\phi)}{\rho} + \frac{\partial f}{\partial \rho}\frac{\cos^2(\phi)}{\rho} \\ &\quad + \frac{\partial^2 f}{\partial \rho \partial \phi}\frac{\sin(\phi)\cos(\phi)}{\rho} + \frac{\partial^2 f}{\partial \phi^2}\frac{\cos^2(\phi)}{\rho^2} - \frac{\partial f}{\partial \phi}\frac{2\cos(\phi)\sin(\phi)}{\rho^2}\end{aligned}. \tag{19}$$

And, of course, we also trivially have

$$\frac{\partial^2 f}{\partial z^2} = \frac{\partial^2 f}{\partial z^2}. \tag{20}$$

Putting Eqs. (18) – (20) together then gives us the fairly simple result

$$\begin{aligned}\nabla^2 f &= \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \\ &= \frac{\partial^2 f}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial f}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2}\end{aligned}. \tag{21}$$

Thus, in cylindrical coordinates the wave equation becomes

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \frac{\partial^2 q}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial q}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 q}{\partial \phi^2} + \frac{\partial^2 q}{\partial z^2} \tag{22}$$

where now $q = q(\rho, \phi, z, t)$.

II. Separation of Variables

To look for separable solutions to the wave equation in cylindrical coordinates we posit a product solution

$$q(\rho, \phi, z, t) = R(\rho)\Phi(\phi)Z(z)T(t). \tag{23}$$

Substituting this into Eq. (22) produces

$$\frac{1}{c^2}R\Phi Z T'' = R''\Phi Z T + \frac{1}{\rho}R'\Phi Z T + \frac{1}{\rho^2}R\Phi'' Z T + R\Phi Z'' T. \tag{24}$$

[1] Notice that Eq. (19) is the same as Eq. (18) with $\sin(\phi) \to \cos(\phi)$ and $\cos(\phi) \to -\sin(\phi)$.

If, as in the case of Cartesian coordinates we now divide by q, which is now written as $R\Phi ZT$, this reduces to

$$\frac{1}{c^2}\frac{T''}{T}=\left(R''+\frac{1}{\rho}R'\right)\frac{1}{R}+\frac{1}{\rho^2}\frac{\Phi''}{\Phi}+\frac{Z''}{Z}. \tag{25}$$

Next time we shall look at the four ordinary differential equations that are equivalent to Eq. (25). Three of these equations will be rather simple (again, essentially harmonic-oscillator equations), but one of them [for $R(\rho)$] will be a new equation. Its solutions are known as Bessel Functions.

Exercises

***20.1** Derive Eqs. (16) and (17). That is, using the chain rule show that $\frac{\partial^2\rho}{\partial x^2}=\frac{\sin^2(\phi)}{\rho}$ and $\frac{\partial^2\phi}{\partial x^2}=\frac{2\cos(\phi)\sin(\phi)}{\rho^2}$.

***20.2** In these lecture notes we have derived the wave equation in cylindrical coordinates by thinking of a function f as a function of x, y, and z through the variables ρ, ϕ, and z, specifically $f=f[\rho(x,y),\phi(x,y),z(z)]$. We can just as easily think of the reverse situation where $f=f[x(\rho,\phi),y(\rho,\phi),z(z)]$. Consider such a function where f is only a function of the distance from the z axis, $\rho=\sqrt{x^2+y^2}$. That is $f=f(\rho)=f\left(\sqrt{x^2+y^2}\right)$. For such a function show that $\partial f/\partial\phi=0$

(**a**) directly in cylindrical coordinates $f=f(\rho)$ and

(**b**) using the chain rule starting with $f=f\left(\sqrt{x^2+y^2}\right)$.

Separation of Variables in Cylindrical Coordinates

Overview and Motivation: Today we look at separable solutions to the wave equation in cylindrical coordinates. Three of the resulting ordinary differential equations are again harmonic-oscillator equations, but the fourth equation is our first foray into the world of special functions, in this case Bessel functions. We then graphically look at some of these separable solutions.

Key Mathematics: More separation of variables; Bessel functions.

I. Cylindrical-Coordinates Separable Solutions

Last time we assumed a product solution $q(\rho,\phi,z,t)=R(\rho)\Phi(\phi)Z(z)T(t)$ to the cylindrical-coordinate wave equation

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2}=\frac{\partial^2 q}{\partial \rho^2}+\frac{1}{\rho}\frac{\partial q}{\partial \rho}+\frac{1}{\rho^2}\frac{\partial^2 q}{\partial \phi^2}+\frac{\partial^2 q}{\partial z^2}, \tag{1}$$

which allowed us to transform Eq. (1) into

$$\frac{1}{c^2}\frac{T''}{T}=\left(R''+\frac{1}{\rho}R'\right)\frac{1}{R}+\frac{1}{\rho^2}\frac{\Phi''}{\Phi}+\frac{Z''}{Z}. \tag{2}$$

We now go through a separation-of-variable procedure similar to that which we carried out using Cartesian coordinates in Lecture 19. The procedure here is a bit more complicated than with Cartesian coordinates because the variable ρ appears in the Φ''/Φ term. However, as we shall see, the equation is still separable.

A. Dependence on Time

As with Cartesian coordinates, we can again make the argument that the rhs of Eq. (2) is independent of t, and so the lhs of this equation must be constant. Cognizant of the fact that we are interested in solutions that oscillate in time, we call this constant $-k^2$ (where we are thinking of k as real) and so we have

$$\frac{1}{c^2}\frac{T''}{T}=-k^2, \tag{3}$$

which can be rearranged as

$$T''+c^2k^2\,T=0. \tag{4}$$

By now we should recognize this as the harmonic oscillator equation, which has two linearly independent solutions,

$$T_k^{\pm}(t) = T_0 e^{\pm ikct}. \tag{5}$$

And so again we have harmonic time dependence to the separable solution.[1] For the present case it is simplest to assume that k can be positive or negative; thus we really only need one of these solutions. So we simply go with

$$T_k(t) = T_0 e^{ikct}. \tag{6}$$

B. Dependence on z

Using Eq. (3), the lhs of Eq. (2) can replaced with $-k^2$, which gives, after a small bit of rearranging,

$$-k^2 - \frac{Z''}{Z} = \left(R'' + \frac{1}{\rho} R' \right) \frac{1}{R} + \frac{1}{\rho^2} \frac{\Phi''}{\Phi}. \tag{7}$$

Notice that the rhs of Eq. (7) is independent of z. Thus the lhs is constant, which we call $-a^2$.[2] We thus have

$$-k^2 - \frac{Z''}{Z} = -a^2, \tag{8}$$

which can be rearranged as

$$Z'' + (k^2 - a^2) Z = 0, \tag{9}$$

which, yet again, is the harmonic oscillator equation! The solutions are

$$Z_{k,a}^{\pm} = Z_0 e^{\pm i\sqrt{k^2 - a^2} z}. \tag{10}$$

Although k and a can be any complex numbers, let's consider the case where both k^2 and a^2 are real and positive. Then these solutions oscillate if $k^2 > a^2$, exponentially grow and decay if $k^2 < a^2$, and are constant if $k^2 = a^2$. Note that here, because the square root is always taken as positive, we need to keep both the positive-sign and negative-sign solutions. We can, however, assume that $a \geq 0$.

[1] It should perhaps be obvious that this will always be the case for separable solutions to the wave equation.

[2] Why not? We can call the constant anything we want. It just so happens that $-a^2$ is convenient.

C. Dependence on ϕ

Using Eq. (8), the lhs of Eq. (7) can be replaced with $-a^2$, which gives us

$$-a^2 = \left(R'' + \frac{1}{\rho} R' \right) \frac{1}{R} + \frac{1}{\rho^2} \frac{\Phi''}{\Phi}. \tag{11}$$

To separate the ρ and ϕ dependence this equation can be rearranged as

$$-\frac{\Phi''}{\Phi} = \left(R'' + \frac{1}{\rho} R' \right) \frac{\rho^2}{R} + \rho^2 a^2. \tag{12}$$

Because each side only depends on one independent variable, both sides of this equation must be constant. This gives us our third separation constant, which we call n^2. The equation for Φ we can then write as

$$\Phi'' + n^2 \Phi = 0, \tag{13}$$

which is again the harmonic oscillator equation. The solutions to Eq. (13) are

$$\Phi_n^{\pm} = \Phi_0 e^{\pm in\phi}. \tag{14}$$

Now we need to use a little physics. Because we expect any physical solution to have the same value for $\phi = 0$ and $\phi = 2\pi$ we must have (for the Φ_n^+ solution)

$$e^0 = e^{in2\pi}, \tag{15}$$

or

$$1 = e^{in2\pi} \tag{16}$$

Using Euler's relation, it is easy to see that Eq. (16) requires that n be an integer. Now because n can be a positive or negative integer, we do not need to explicitly keep up with the Φ_n^- solution, and so we write for the ϕ dependence

$$\Phi_n = \Phi_0 e^{in\phi}, \qquad n = 0, \pm 1, \pm 2, \ldots \tag{17}$$

D. Dependence on ρ

We are now left with one last equation. Also setting the rhs of Eq. (12) equal to n^2 and doing a bit of rearranging yields

$$\rho^2 R'' + \rho R' + \left(a^2\rho^2 - n^2\right)R = 0 \tag{18}$$

This is definitely *not* the harmonic oscillator equation! Its solutions are well know functions, but to see what the solutions to Eq. (18) are we need to put it in "standard" form, which is a form that we can look up in a book such as *Handbook of Mathematical Functions* by Abramowitz and Stegun (the definitive, concise book on special functions, which has been updated an is available online as the *NIST Digital Library of Mathematical Functions*).

To put Eq. (18) in standard form, we make the substitution $s = a\rho$. Now the substitution would be trivial, except that because Eq. (18) is a differential equation in the independent variable ρ, we need to change the derivatives in Eq. (18) to derivatives in s. As usual we do this using the chain rule. If we now think of $R(\rho)$ as a function of ρ through the new independent variable s, i.e., as $R[s(\rho)]$, then using

$$\frac{dR}{d\rho} = \frac{dR}{ds}\frac{ds}{d\rho} = \frac{dR}{ds}a \tag{19a}$$

and

$$\frac{d^2R}{d\rho^2} = \frac{d}{d\rho}\left(\frac{dR}{ds}\frac{ds}{d\rho}\right) = \frac{d^2R}{ds^2}\left(\frac{ds}{d\rho}\right)^2 + \frac{dR}{ds}\frac{d^2s}{d\rho^2} = \frac{d^2R}{ds^2}a^2 . \tag{19b}$$

we can rewrite Eq. (18) as

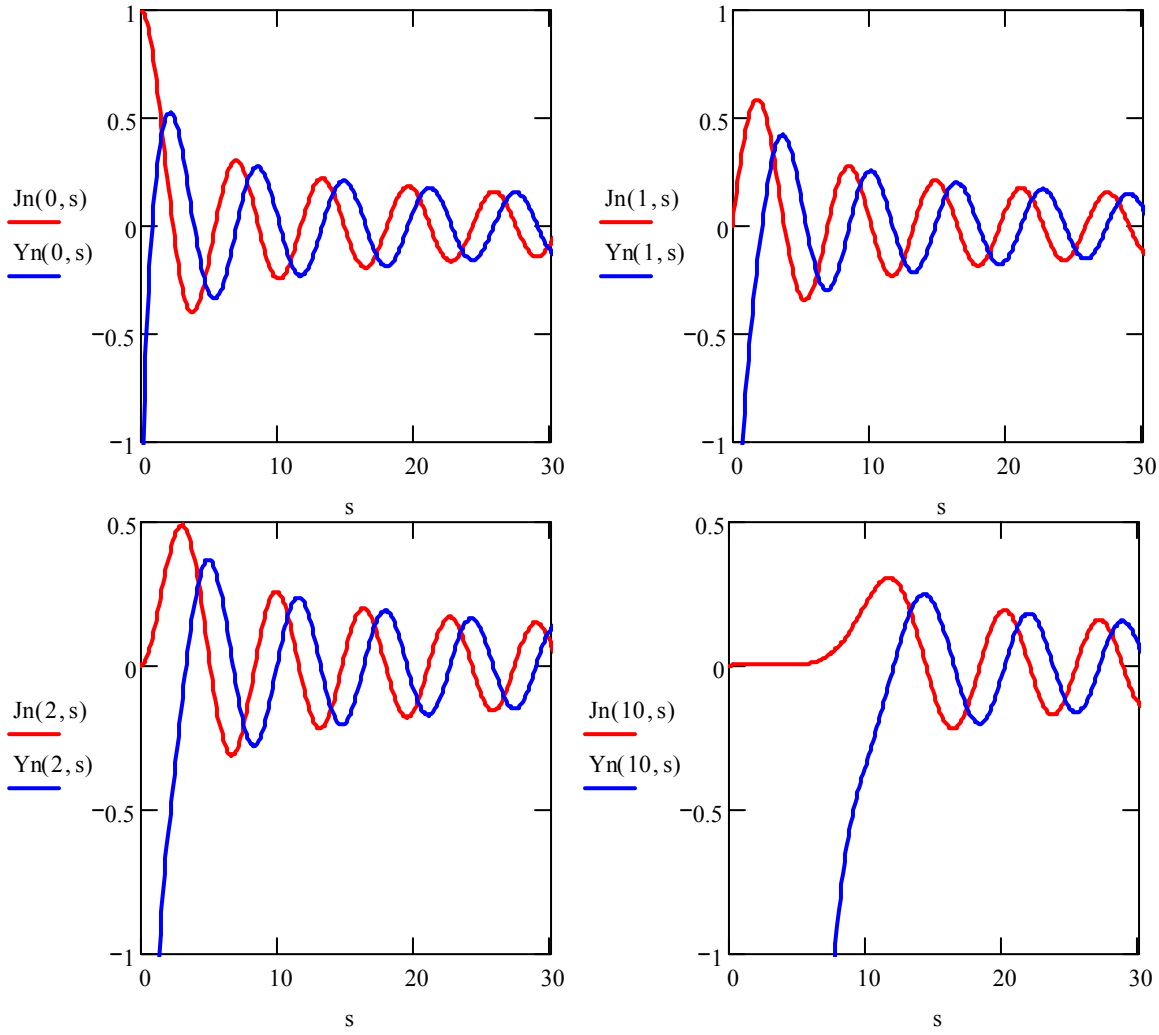
$$\left(\frac{s}{a}\right)^2 R''(s)a^2 + \frac{s}{a}R'(s)a + \left(s^2 - n^2\right)R(s) = 0 . \tag{20}$$

where we now emphasize that $R = R(s)$. Equation (20) obviously simplifies to

$$s^2R''(s) + s\,R'(s) + \left(s^2 - n^2\right)R(s) = 0 . \tag{21}$$

This equation is know as **Bessel's equation**. It's two linearly independent solutions are known as **Bessel functions** $J_n(s)$ and **Neumann functions** $Y_n(s)$. Sometimes the functions $J_n(s)$ and $Y_n(s)$ are called **Bessel functions of the first and second kind**, respectively. The subscript n is know as the **order** of the Bessel function Although one can define Bessel functions of non-integer order, one outcome of the Φ equation is that n is an integer, so we only need deal with integer-order Bessel functions for this problem.

The following figure plots both $J_n(s)$ and $Y_n(s)$ for several values of (positive) n.



There are several facts about Bessel functions that are worth noting, some of which can be discerned from these graphs:

(*i*) $J_0(0)=1$; $J_n(0)=0$, $n\neq 0$. $Y_n(s)$ diverges as $s\to 0$. Also notice the behavior of these functions as $s\to 0$ for increasing n: the functions $J_n(s)$ converge more rapidly while the functions $Y_n(s)$ diverge more rapidly.

(*ii*) $J_n(s)$ and $Y_n(s)$ oscillate with decreasing amplitude as $s\to\infty$.

(*iii*) It is customary to define $J_{-n}=(-1)^n J_n$ and $Y_{-n}=(-1)^n Y_n$. (Notice that the Bessel equation only depends upon n^2, so the $-n$ solution must be essentially the same as the $+n$ solution.)

(*iv*) Bessel functions have the series representation

$$J_n(s) = \sum_{m=0}^{\infty} \frac{(-1)^m}{2^{2m}\, m!\, \Gamma(m+n+1)} \left(\frac{s}{2}\right)^{2m+n}, \tag{22}$$

where

$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t}\, dt \tag{23}$$

is the **Gamma** function. Note that for integer x, $\Gamma(x+1) = x! = x(x-1)(x-2)\cdots 1$.

$$(v) \quad Y_n(s) = \lim_{n' \to n} \frac{J_{n'}(s)\cos(n'\pi) - J_{-n'}(s)}{\sin(n'\pi)} \tag{24}$$

More entertaining facts about Bessel functions can be found in the *NIST Digital Library of Mathematical Functions*.

Now because $s = a\rho$, the solutions to Eq. (18) are thus simply $J_n(a\rho)$ and $Y_n(a\rho)$. That is, we have the two linearly independent results

$$R^J_{n,a}(\rho) = R_J\, J_n(a\rho) \quad \text{and} \quad R^Y_{n,a}(\rho) = R_Y\, Y_n(a\rho). \tag{25a) – (25b)}$$

II. Separable Solutions

Let's put all of this analysis together and write down our separable solutions. Let's further assume that (1) we want the z dependence of the solution to oscillate (or at least not either grow or decay exponentially) and (2) we are only interested in solutions that remain finite as $\rho \to 0$. We then have the following pieces to our separable solution

$$T_k(t) = T_0 e^{ikct}, \qquad -\infty < k < \infty \tag{25a}$$

$$Z^{\pm}_{k,a} = Z_0 e^{\pm i\sqrt{k^2 - a^2}\, z}, \qquad a \le |k| \tag{25b}$$

$$\Phi_n = \Phi_0 e^{in\phi}, \qquad n = 0, \pm 1, \pm 2, \ldots \tag{25c}$$

$$R_{a,n}(\rho) = R_0\, J_n(a\rho). \tag{25d}$$

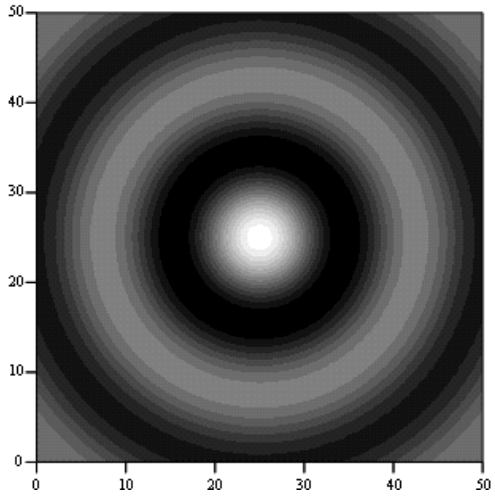
Putting all of Eq. (24) together we can write our separable solutions as

$$q^{\pm}_{n,a,k}(\rho,\phi,z,t) = C^{\pm}_{n,a,k}\, J_n(a\rho)\, e^{in\phi}\; e^{\pm i\sqrt{k^2-a^2}\,z}\; e^{ikct}\,. \tag{26}$$

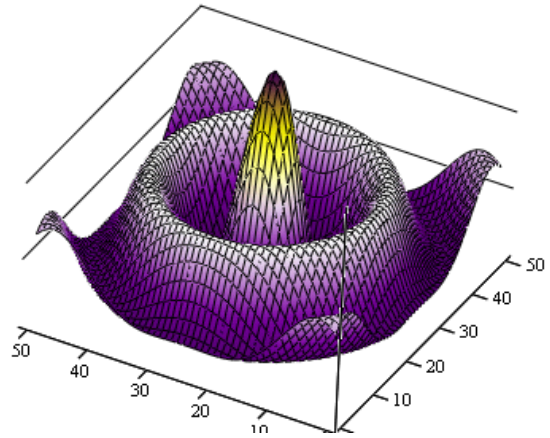
Let's look at some graphs of some of these functions. For simplicity we look at functions that have no z dependence. From Eq. (26) we see that these are solutions where $k = \pm a$. With this constraint we can write Eq. (6) as

$$q_{n,a,\pm a}(\rho,\phi,z,t) = C_{n,a,\pm a}\, J_n(a\rho)\, e^{in\phi}\; e^{\pm iact}\,. \tag{27}$$

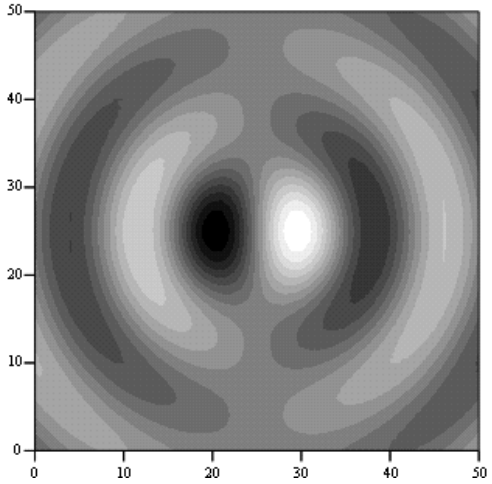
The following pictures show graphs (with $a = 1$) of $\mathrm{Re}\left[q_{0,a,a}(\rho,\phi,z,0)\right] = J_0(a\rho)$, $\mathrm{Re}\left[q_{1,a,a}(\rho,\phi,z,0)\right] = J_1(a\rho)\cos(\phi)$, and $\mathrm{Re}\left[q_{2,a,a}(\rho,\phi,z,0)\right] = J_2(a\rho)\cos(2\phi)$.



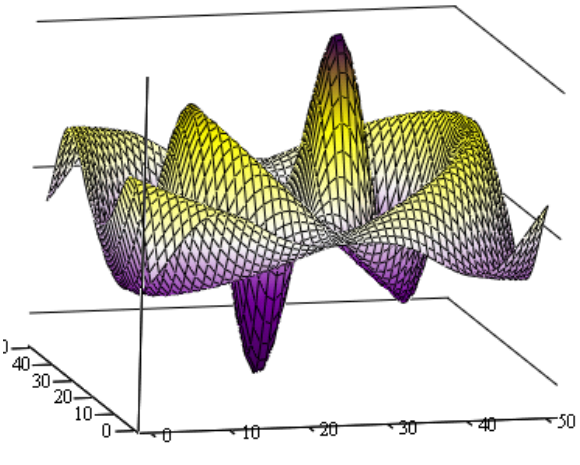
$\mathrm{Re}(q_0)$



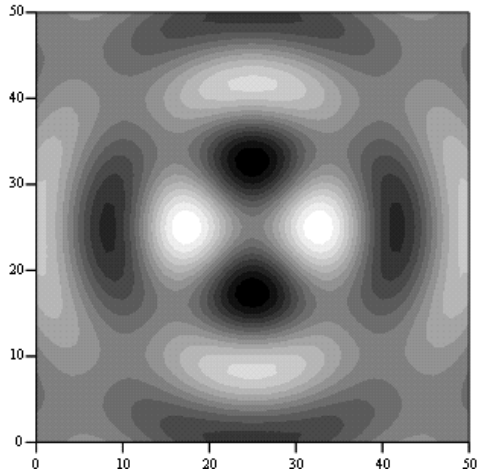
$\mathrm{Re}(q_0)$



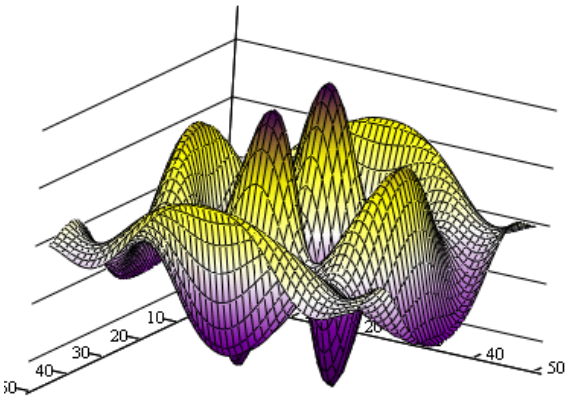
$\mathrm{Re}(q_1)$



$\mathrm{Re}(q_1)$



Re(q2)



Re(q2)

For the moment, this ends our discussion of cylindrical coordinates. In the next lecture we move on to studying the wave equation in spherical-polar coordinates.

Exercises

*21.1 Dispersion Relation.

Consider the solution $q^{\pm}_{n,a,k}(\rho,\phi,z,t) = C^{\pm}_{n,a,k}\left[J_n(a\rho)+iY(a\rho)\right]\cos(n\phi)\,e^{\pm i\sqrt{k^2-a^2}\,z}\,e^{-ikct}$.
From this equation it is clear that the frequency ω is equal to ck. This looks like there is a dispersion relation, but it is not really clear what k represents in this case. Here we show that if positive, it is essentially the magnitude of a wave vector $\mathbf{k} = k_\rho\hat{\boldsymbol{\rho}} + k_z\hat{\mathbf{z}}$ (where the meanings of the unit vectors should be obvious). To do this we take advantage of the fact that for large s, the Bessel functions have the asymptotic expansions

$$J_n(s) \approx \sqrt{\frac{2}{\pi s}}\cos\left(s - \tfrac{1}{2}n\pi - \tfrac{1}{4}\pi\right) \qquad \text{and} \qquad Y_n(s) \approx \sqrt{\frac{2}{\pi s}}\sin\left(s - \tfrac{1}{2}n\pi - \tfrac{1}{4}\pi\right).$$

(**a**) Using these equations show that component of the wave vector in the ρ direction is $k_\rho = a$.

(**b**) Identify the z component k_z of the wave vector.

(**c**) Then, show that $k_\rho^2 + k_z^2 = k^2$.

*__21.2 Linear Combinations of Bessel Functions__. The Bessel functions of the *third* kind (also known as *Hankel* functions) are defined as

$$H_n^{(1)}(s) = J_n(s) + iY_n(s) \qquad \text{and} \qquad H_n^{(2)}(s) = J_n(s) - iY_n(s).$$

(**a**) Using the asymptotic expansions given in Exercise 21.1, show for large s that

$$H_n^{(1)}(s) \approx \sqrt{\frac{2}{\pi s}} e^{i\left(s - \frac{1}{2}n\pi - \frac{1}{4}\pi\right)} \qquad \text{and} \qquad H_n^{(2)}(s) \approx \sqrt{\frac{2}{\pi s}} e^{-i\left(s - \frac{1}{2}n\pi - \frac{1}{4}\pi\right)}.$$

(**b**) Using the results of (a) describe the behavior of the waves

$$q_{0,a,a}^{(1)}(\rho,\phi,z,t) = H_0^{(1)}(a\rho)\, e^{-iact} \qquad \text{and} \qquad q_{0,a,a}^{(2)}(\rho,\phi,z,t) = H_0^{(2)}(a\rho)\, e^{-iact}.$$

for large ρ (assuming that $a > 0$) (That is, are they standing or traveling waves, etc).

Separation of Variables in Spherical Coordinates

Overview and Motivation: We look at separable solutions to the wave equation in one more coordinate system – spherical (polar) coordinates. These coordinates are most useful for solving problems with spherical symmetry.

Key Mathematics: Spherical coordinates, the chain rule, and associated Legendre functions (including Legendre polynomials).

I. Spherical Coordinates and the Wave Equation

As in the case of the cylindrical-coordinates version of the wave equation, our first job will be to express the Laplacian ∇^2 in spherical coordinates (r,θ,ϕ), which are defined in terms of Cartesian coordinates (x,y,z) as

$$r = \sqrt{x^2 + y^2 + z^2}\,, \tag{1a}$$

$$\theta = \arccos\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \tag{1b}$$

$$\phi = \arctan\left(\frac{y}{x}\right). \tag{1c}$$

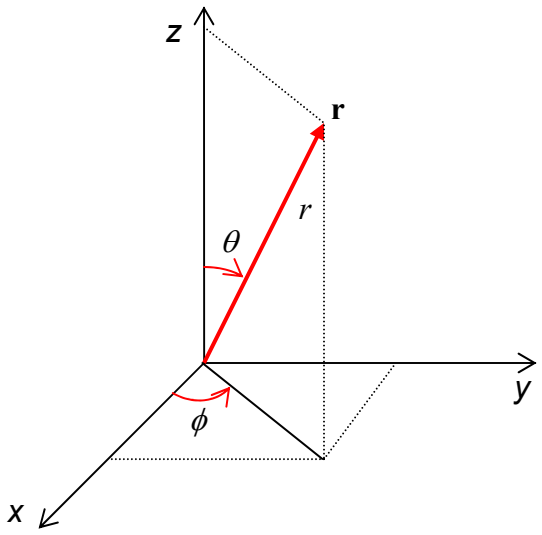
The diagram at the top of the next page graphically illustrates these coordinates for the vector $\mathbf{r}$. The coordinate r is the length of $\mathbf{r}$; the coordinate θ (known as the **polar angle**) is the angle of the vector $\mathbf{r}$ from the z axis; the coordinate ϕ (known as the **azimuthal angle**) is the angle of the xy-plane projection of $\mathbf{r}$ from the x axis to the y axis. Notice that the coordinate ϕ is also used in cylindrical coordinates.

To write $\nabla^2 f$ (where f is some function of r, θ, and ϕ) in spherical coordinates we go through the same procedure as we did for cylindrical coordinates. We think of f as a function of x, y, and z through the new coordinates r, θ, and ϕ

$$f = f\left[r(x,y,z),\theta(x,y,z),\phi(x,y,z)\right]$$

and then re-express

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \tag{2}$$



in terms of the new coordinates using the chain rule. For example, to re-express the x-derivative term we first use the chain rule to write

$$\frac{\partial f}{\partial x}=\frac{\partial f}{\partial r}\frac{\partial r}{\partial x}+\frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x}+\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}. \tag{3}$$

Using Eq. (3) we can then express the second derivative as

$$\frac{\partial^2 f}{\partial x^2}=\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)=\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial r}\frac{\partial r}{\partial x}+\frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x}+\frac{\partial f}{\partial \phi}\frac{\partial \phi}{\partial x}\right), \tag{4}$$

and then using the chain rule again we can write

$$\begin{aligned}\frac{\partial^2 f}{\partial x^2}=&\left(\frac{\partial^2 f}{\partial r^2}\frac{\partial r}{\partial x}+\frac{\partial^2 f}{\partial \theta \partial r}\frac{\partial \theta}{\partial x}+\frac{\partial^2 f}{\partial \phi \partial r}\frac{\partial \phi}{\partial x}\right)\frac{\partial r}{\partial x}+\frac{\partial f}{\partial r}\frac{\partial^2 r}{\partial x^2}\\&+\left(\frac{\partial^2 f}{\partial r\partial \theta}\frac{\partial r}{\partial x}+\frac{\partial^2 f}{\partial \theta^2}\frac{\partial \theta}{\partial x}+\frac{\partial^2 f}{\partial \phi \partial \theta}\frac{\partial \phi}{\partial x}\right)\frac{\partial \theta}{\partial x}+\frac{\partial f}{\partial \theta}\frac{\partial^2 \theta}{\partial x^2}\\&+\left(\frac{\partial^2 f}{\partial r\partial \phi}\frac{\partial r}{\partial x}+\frac{\partial^2 f}{\partial \theta \partial \phi}\frac{\partial \theta}{\partial x}+\frac{\partial^2 f}{\partial \phi^2}\frac{\partial \phi}{\partial x}\right)\frac{\partial \phi}{\partial x}+\frac{\partial f}{\partial \phi}\frac{\partial^2 \phi}{\partial x^2}\end{aligned}. \tag{5}$$

Pretty ugly, eh? Actually, if you scrutinize Eq. (5) you will see that there is a bit of symmetry present: switching any of the spherical coordinates results in the same equation.

Although we will not go through the rest of the procedure, you should recall that there are two types of terms in Eq. (5). There are derivatives of f with respect to the new variable (which remain unchanged) and there are derivatives of the new variables with respect to the old variable x. We must calculate these second type of derivatives and then express them in terms of the new variables using Eq. (1). If we go through this procedure for all three terms in the Laplacian and sum everything up, we end up with the spherical-coordinates expression for the wave equation

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial q}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left[\sin(\theta)\frac{\partial q}{\partial\theta}\right] + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2 q}{\partial\phi^2} \tag{6}$$

II. Separation of Variable in Spherical Coordinates

As before we look for separable solutions to the wave equation by assuming that we can write $q(r,\theta,\phi,t)$ as a product solution

$$q(r,\theta,\phi,t) = R(r)\Theta(\theta)\Phi(\phi)T(t). \tag{7}$$

Substituting this into Eq. (6) and dividing the result by $R(r)\Theta(\theta)\Phi(\phi)T(t)$ yields

$$\frac{1}{c^2}\frac{T''}{T} = \frac{1}{r^2R}\left(r^2R'\right)' + \frac{1}{r^2\sin(\theta)}\frac{1}{\Theta}\left[\sin(\theta)\Theta'\right]' + \frac{1}{r^2\sin^2(\theta)}\frac{\Phi''}{\Phi}. \tag{8}$$

A. Dependence on Time

As with Cartesian and cylindrical coordinates, we again make the argument that the rhs of Eq. (8) is independent of t, and so the lhs of this equation must be constant. As with cylindrical coordinates we call this constant $-k^2$ (where we are thinking of k as real) and so we again have

$$T'' + c^2k^2T = 0, \tag{9}$$

which has the two linearly independent solutions,

$$T_k^{\pm}(t) = T_0e^{\pm ikct}. \tag{10}$$

B. Dependence on ϕ

Equating the rhs of Eq. (8) to $-k^2$, multiplying by $r^2\sin^2(\theta)$, and doing some rearranging of terms gives us

$$\frac{\Phi''}{\Phi} = -k^2 r^2 \sin^2(\theta) - \frac{\sin^2(\theta)}{R}\left(r^2 R'\right)' - \frac{\sin(\theta)}{\Theta}\left[\sin(\theta)\Theta'\right]', \tag{11}$$

which separates out the ϕ dependence from r and θ. Equating the lhs of Eq. (11) to the constant $-m^2$ gives us the equation for Φ,[1]

$$\Phi'' + m^2\Phi = 0, \tag{12}$$

which, yet again, is the harmonic oscillator equation. Equation (12) has the solutions

$$\Phi_m^{\pm}(\phi) = \Phi_0 e^{\pm im\phi}. \tag{13}$$

Again, because we require continuous solutions as a function of ϕ, we must restrict m to integer values, $m = 0, \pm 1, \pm 2, \ldots$. Note that the dependence on ϕ is exactly the same as in the cylindrical-coordinates case.

C. Dependence on θ.

The last variable that we will deal with today is the polar angle θ. If we now equate the rhs of Eq. (11) to $-m^2$, divide by $\sin^2(\theta)$, and do a bit of rearranging, we end up with

$$\frac{1}{\sin(\theta)\Theta}\left[\sin(\theta)\Theta'\right]' - \frac{m^2}{\sin^2(\theta)} = -\frac{1}{R}\left(r^2 R'\right)' - k^2 r^2, \tag{14}$$

which separates the θ and r variables. Each side of this equation is a constant, which by convention is taken to be $-l(l+1)$. This results in the differential equation for $\Theta(\theta)$

$$\frac{1}{\sin(\theta)}\left[\sin(\theta)\Theta'\right]' + \left[l(l+1) - \frac{m^2}{\sin^2(\theta)}\right]\Theta = 0 \tag{15}$$

This is definitely not the harmonic oscillator equation! It is however, close to the standard form of another well known equation. To put Eq. (15) in this standard form we make the change of variables $s(\theta) = \cos(\theta)$. We now think of Θ as a function of θ through the variable s as $\Theta = \Theta[s(\theta)]$, and we write the derivatives of Θ as

[1] You may ask why we do we use $-m^2$ for spherical coordinates when we used $-n^2$ for cylindrical coordinates? I have no idea.

$$\frac{d\Theta}{d\theta}=\frac{d\Theta}{ds}\frac{ds}{d\theta}=\frac{d\Theta}{ds}\left[-\sin(\theta)\right]=\frac{d\Theta}{ds}\left[-\sqrt{1-s^2}\right] \tag{16a}$$

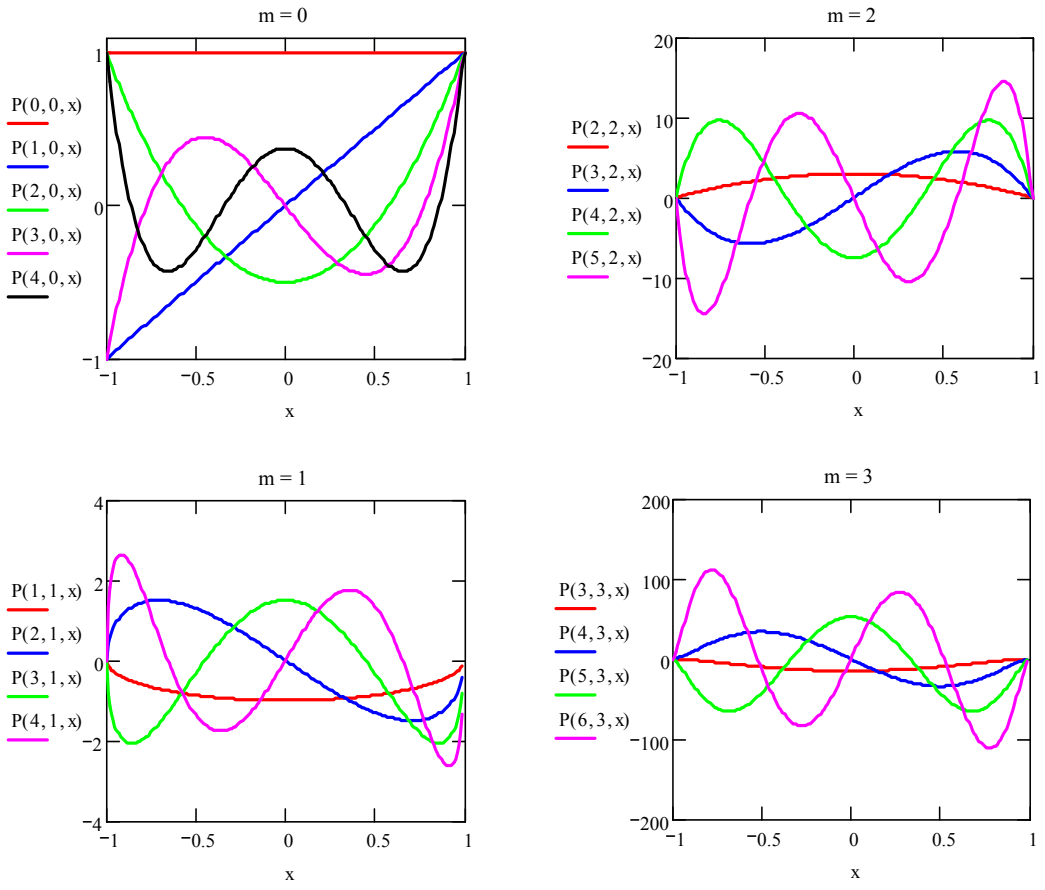
and

$$\begin{aligned}\frac{d^2\Theta}{d\theta^2}&=\frac{d}{d\theta}\left(\frac{d\Theta}{ds}\frac{ds}{d\theta}\right)=\frac{d^2\Theta}{ds^2}\left(\frac{ds}{d\theta}\right)^2+\frac{d\Theta}{ds}\frac{d^2s}{d\theta^2}\\&=\frac{d^2\Theta}{ds^2}\left(1-s^2\right)+\frac{d\Theta}{ds}\left[-s\right]\end{aligned}. \tag{16b}$$

Substituting Eq. (16) into Eq. (15) yields, after a bit of algebra,

$$\left(1-s^2\right)\Theta''(s)-2s\,\Theta'(s)+\left[l(l+1)-\frac{m^2}{1-s^2}\right]\Theta(s)=0\,. \tag{17}$$

This equation is known as the **associated Legendre equation**. As with all second-order linear, ordinary differential equations, there are two linearly independent solutions. These solutions are know as **associated Legendre functions of the first**



and second kind, which are denoted $P_l^m(s)$ and $Q_l^m(s)$, respectively. Usually we are interested in only the $P_l^m(s)$ solutions because the $Q_l^m(s)$ solutions diverge as $s \to \pm 1$.

The figure on the previous page plots some of the $P_l^m(s)$ functions for various values of l and m. Notice that these functions are plotted for $-1 \le s \le 1$ because this corresponds to $0 \le \theta \le \pi$, the range of the polar angle θ. The following statements summarize some key feature of the associate Legendre functions, some of which are evident in the figure.

(*i*) For the $P_l^m(s)$ solutions to Eq. (17) to remain finite, the parameter l must be an integer and m, which is already an integer, must satisfy $|m| \le l$. (You are already likely familiar with this result from quantum mechanics, where the angular parts of the separable solutions of the Schrödinger in spherical coordinates are identical to the solutions here.)

(*ii*) For $m = 0$ (azimuthal symmetry) the solutions $P_l(s) \equiv P_l^0(s)$ are known as **Legendre polynomials**. These functions are polynomials in s of order l. The first four Legendre polynomials are

$$P_0(s) = 1, \qquad P_1(s) = s, \qquad P_2(s) = \frac{1}{2}\left(3s^2 - 1\right), \qquad P_3(s) = \frac{1}{2}\left(5s^3 - 3s\right) \qquad \text{(18a)} - \text{(18d)}$$

(*iii*) A nice simple formula for calculating the Legendre polynomials, known as **Rodrigues' formula**, is

$$P_l(s) = \frac{1}{2^l\, l!}\frac{d^l\left(s^2 - 1\right)^l}{ds^l} \tag{19}$$

(*iv*) For the associated Legendre functions Rodrigues' formula generalizes to

$$P_l^m(s) = \frac{1}{2^l\, l!}\left(1 - s^2\right)^{|m|/2}\frac{d^{|m|+l}}{ds^{|m|+l}}\left(s^2 - 1\right)^l. \tag{20}$$

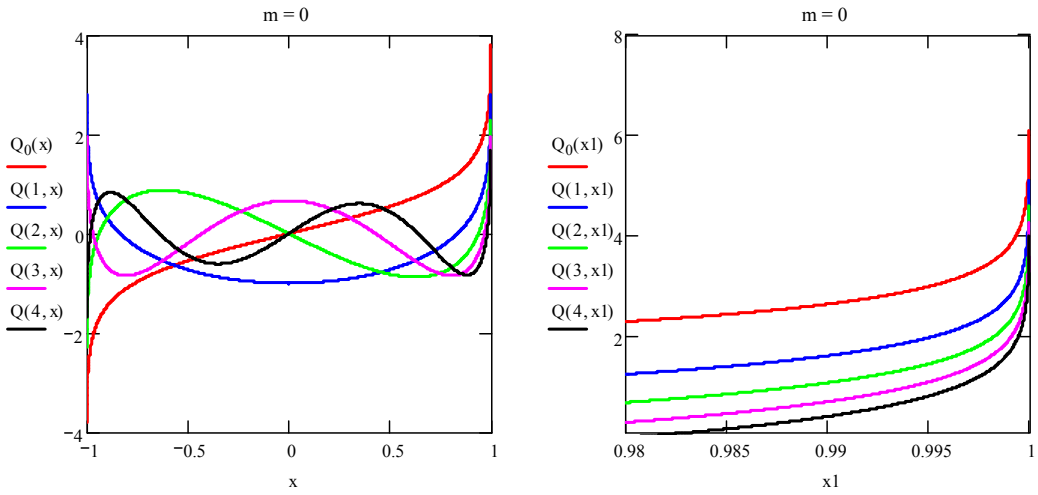
(*v*) The first few $m = 0$ Legendre functions of the second kind can be written as

$$Q_0(s) = \frac{1}{2}\ln\left(\frac{1+s}{1-s}\right), \quad Q_1(s) = \frac{s}{2}\ln\left(\frac{1+s}{1-s}\right) - 1, \quad Q_2(s) = \frac{3s^2 - 1}{4}\ln\left(\frac{1+s}{1-s}\right) - \frac{3s}{2}. \quad \text{(21a)} - \text{(21c)}$$

(*vi*) For $l \geq 1$ the $m = 0$ Legendre functions of the second kind can be expressed in terms of the Legendre functions of the first kind as

$$Q_l(s) = \frac{1}{2} P_l(s) \ln\left(\frac{1+s}{1-s}\right) - \sum_{m=1}^{l} \left[\frac{1}{m} P_{m-1}(s) P_{l-m}(s)\right]. \tag{22}$$

The following figure plots the first few of these functions. Notice that they all diverge as $|s| \to 1$, although because the divergence involves the logarithm function, the divergence is very slow, as the graph on the rhs of the figure illustrates.

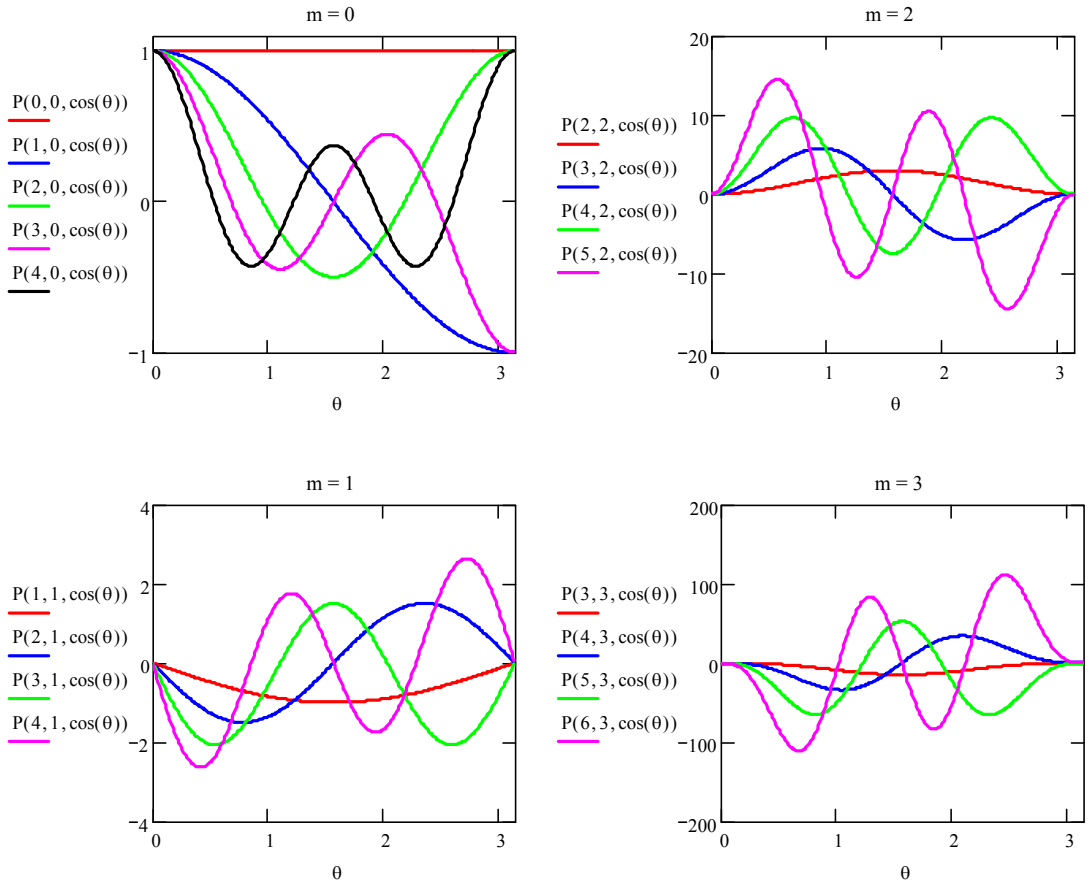


As with the Bessel functions, more entertaining facts about associated Legendre functions can be found in *Handbook of Mathematical Functions* by Abramowitz and Stegun or in the online *NIST Digital Library of Mathematical Functions*.

Now that we have some idea of the behavior of these functions, we can get back to our solution of the wave equation. Because $s = \cos(\theta)$ the solutions to Eq. (15) are

$$\Theta^P_{l,m}(\theta) = \Theta_P P_l^m(\cos(\theta)) \quad \text{and} \quad \Theta^Q_{l,m}(\theta) = \Theta_Q Q_l^m(\cos(\theta)), \tag{23}$$

(or some linear combination of the two solutions) Because they remain finite, we are usually exclusively interested in solutions involving Legendre functions of the first kind. The figure at the top of the next page plots some of the $P_l^m(\cos(\theta))$ functions as a function of θ. Notice that they are similar, but not identical to the functions plotted on p. 5.



Exercises

*__22.1__ Calculate the change-of-coordinates derivatives $\partial r/\partial x$, $\partial\theta/\partial x$, and $\partial\phi/\partial x$ and express them as functions of the new variables.

*__22.2__ Consult the figure on p. 5. For the function $P_l^m(s)$, how many zero crossings of are there for $-1 < s < 1$? That is, deduce the formula for the number of zero crossings as a function of l and m.

*__22.3__ The Legendre polynomials $P_l^0(x)$ can be used as a set of orthogonal basis functions on the interval $-1 \le x \le 1$. Using the standard definition of the inner product, show that P_0, P_1, and P_2 are all orthogonal. Find normalized versions of each of these functions.

*__22.4__ Using Eq. (7), derive Eq. (8) from Eq. (6).

Spherical Coordinates II / A Boundary Value Problem / Separation of Variables Summary

Overview and Motivation: We look at the fourth differential equation that arises in the separable solution to the spherical-coordinates wave equation. We then review the separable solutions in all three coordinate systems – Cartesian, cylindrical, and spherical. Finally, we use a separable solution to find the normal modes of a drumhead.

Key Mathematics: More separation of variables, spherical Bessel functions, and normal modes in polar coordinates.

I. Separation of Variables in Spherical Coordinates (continued)

Last time we began our search for separable solutions to the wave equation in spherical coordinates,

$$\frac{1}{c^2}\frac{\partial^2 q}{\partial t^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial q}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left[\sin(\theta)\frac{\partial q}{\partial\theta}\right] + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2 q}{\partial\phi^2}. \tag{1}$$

We assumed a solution of the form $q(r,\theta,\phi,t) = R(r)\Theta(\theta)\Phi(\phi)T(t)$ and then solved three ordinary differential equations, which gave us the three functions $T(t)$, $\Phi(\phi)$, and $\Theta(\theta)$. Because each of these differential equations is second-order, linear, and homogeneous, there are two linearly independent solutions that can be (linearly) combined to produce the most general form of each solution. For the functions $T(t)$, $\Phi(\phi)$, and $\Theta(\theta)$ the most general forms can be written as

$$T_k(t) = A_k e^{ikct} + B_k e^{-ikct}, \tag{2}$$

$$\Phi_m(\phi) = C_m e^{im\phi} + D_m e^{-im\phi}, \qquad m = 0, 1, 2, \ldots l, \tag{3}$$

$$\Theta_{l,m}(\theta) = E_{l,m}\, P_l^m(\cos(\theta)) + F_{l,m} Q_l^m(\cos(\theta)), \qquad l = 0, 1, 2, \ldots \tag{4}$$

Here A_k, C_m, and $F_{l,m}$, etc. are undetermined constants, and P_l^m and Q_l^m are associated Legendre functions of the first and second kind, respectively.

Let's now look at the $R(r)$ part of $q(r,\theta,\phi,t)$. Looking back at p. 4 of the Lecture 22 notes we see that the ordinary differential equation for $R(r)$ is

$$-l(l+1) = -\frac{1}{R}\left(r^2R'\right)' - k^2r^2, \tag{5}$$

which can be rewritten as

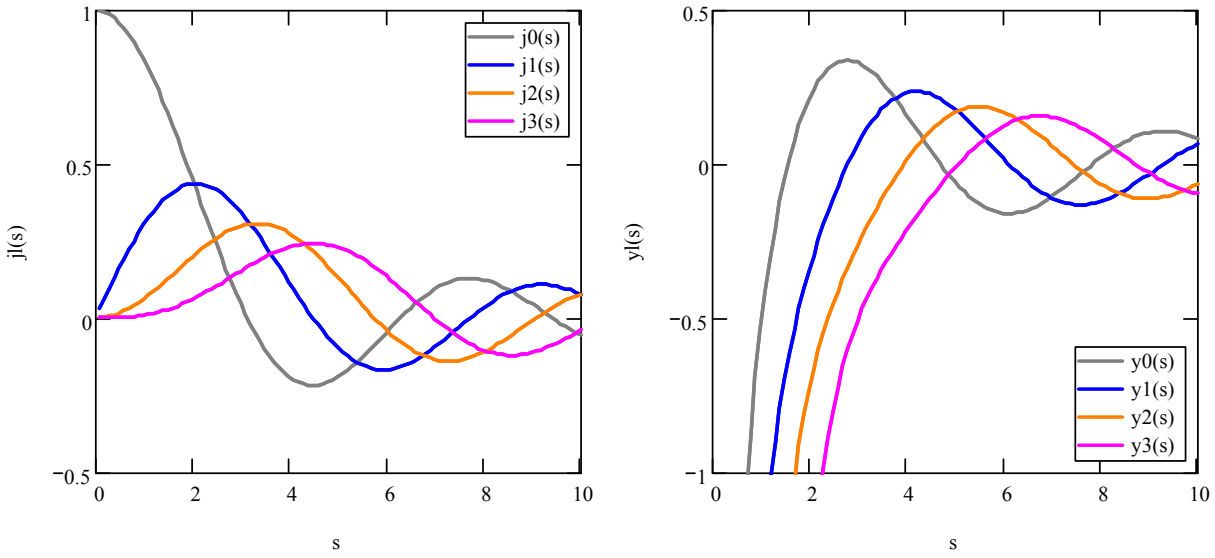
$$r^2R'' + 2rR' + \left[k^2r^2 - l(l+1)\right]R = 0\,. \tag{6}$$

As with some of the other equations that we have looked at, this not quite in standard form. Equation (6) can be put in standard form (in a manner similar to the Bessel equation that arose in cylindrical coordinates) by defining the new independent variable $s = kr$. With this definition (and the chain rule) Eq. (6) can be transformed into

$$s^2R''(s) + 2sR'(s) + \left[s^2 - l(l+1)\right]R(s) = 0\,, \tag{7}$$

where we emphasize that R is now a function of the new variable s. If you look back at Eq. (21) of the Lecture 21 notes (Bessel's equation), you will see that Eq. (7) is quite similar to that equation.

The solutions to Eq. (7) (which are indeed similar to Bessel functions) are known as **spherical Bessel functions**. The spherical Bessel functions of the **first and second kind** are denoted $j_l(s)$ and $y_l(s)$. The following figure plots these functions (for $l = 0,1,2,3$).



The following facts about these functions, some of which can be discerned from the graphs, are worth noting.

(*i*) $j_l(s)$ are finite everywhere; $y_l(s)$ diverge as $s \to 0$. Also notice the behavior of these functions as $s \to 0$ for increasing l: the functions $j_l(s)$ converge more rapidly while the functions $y_l(s)$ diverge more rapidly.

(*ii*) The functions oscillate with decreasing amplitude as $s \to \infty$.

(*iii*) The spherical Bessel functions can be written in terms of (standard) Bessel functions of *noninteger* order as

$$j_l(s) = \sqrt{\tfrac{1}{2}\pi/s}\, J_{l+\frac{1}{2}}(s), \qquad y_l(s) = \sqrt{\tfrac{1}{2}\pi/s}\, Y_{l+\frac{1}{2}}(s) \tag{8a), (8b}$$

(*iv*) The $j_l(s)$ functions have the convenient integral representation[1]

$$j_l(s) = \frac{s^l}{2^{l+1}\Gamma(l+1)} \int_0^\pi \cos[s\cos(\theta)]\sin^{2l+1}(\theta)\, d\theta\,. \tag{9}$$

(*v*) The first three $j_l(s)$'s and $y_l(s)$'s can be represented in terms of sine and cosine functions as

$$j_0(s) = \frac{\sin(s)}{s}, \qquad y_0(s) = -\frac{\cos(s)}{s}, \tag{10a), (10b}$$

$$j_1(s) = \frac{\sin(s)}{s^2} - \frac{\cos(s)}{s}, \qquad y_1(s) = -\frac{\cos(s)}{s^2} - \frac{\sin(s)}{s}, \tag{10c), (10d}$$

$$j_2(s) = \left(\frac{3}{s^3} - \frac{1}{s}\right)\sin(s) - \frac{3}{s^2}\cos(s), \qquad y_2(s) = -\left(\frac{3}{s^3} - \frac{1}{s}\right)\cos(s) - \frac{3}{s^2}\sin(s). \tag{10e), (10f}$$

Similar, although increasingly more complicated, formulae can be derived for higher-order $j_l(s)$'s and $y_l(s)$'s. Notice that the formulae for $y_l(s)$ are identical to the formula for $j_l(s)$ with the changes $\sin(s) \to -\cos(s)$ and $\cos(s) \to \sin(s)$.

Let's now get back to our solution to the wave equation. Because $s = kr$, the solution to Eq. (6) [the equation for $R(r)$], can be generally written as

[1] At least Eq. (9) can be convenient when using a computer mathematic program such as Mathcad. In fact, you can use Eq. (9) and Mathcad to generate the formulae for $j_l(s)$ in Eq. (10).

$$R_{k,l}(r) = G_{k,l} j_l(kr) + H_{k,l} y_l(kr). \tag{11}$$

So putting Eqs. (2), (3), (4), and (11) together we now have the general form of the separable solution in spherical coordinates

$$\begin{aligned} q_{k,l,m}(r,\theta,\phi,t) = &\left[G_{k,l} j_l(kr) + H_{k,l} y_l(kr)\right]\left[E_{l,m} P_l^m(\cos(\theta)) + F_{l,m} Q_l^m(\cos(\theta))\right] \\ &\times \left(C_m e^{im\phi} + D_m e^{-im\phi}\right)\left(A_k e^{ikct} + B_k e^{-ikct}\right) \end{aligned}, \tag{12}$$

where the parameters l and m are specified by $l = 0, 1, 2, \ldots$ and $m = 0, 1, 2, \ldots l$. The parameter k is unspecified.

II. Summary of Separable Solutions

We previously wrote down separable solutions in the other coordinate systems, but never in as general a form as Eq. (12) for spherical coordinates. Let's now do this for the previous coordinate systems. For cylindrical coordinates we can write the general separable solution as

$$\begin{aligned} q_{n,a,k}(\rho,\phi,z,t) = &\left[G_{n,a} J_n(a\rho) + H_{n,a} Y_n(a\rho)\right]\left(E_n e^{in\phi} + F_n e^{-in\phi}\right) \\ &\times \left(C_{k,a} e^{i\sqrt{k^2-a^2}\,z} + D_{k,a} e^{-i\sqrt{k^2-a^2}\,z}\right)\left(A_k e^{ikct} + B_k e^{-ikct}\right) \end{aligned}, \tag{13}$$

where J_n and Y_n are Bessel functions. The parameter n is specified by $n = 0, 1, 2, \ldots$, but the parameters a and k are unspecified. Similarly, for Cartesian coordinates we have[2]

$$\begin{aligned} q_{k_x,k_y,k_z}(x,y,z,t) = &\left(G_{k_x} e^{ik_x x} + H_{k_x} e^{-ik_x x}\right)\left(E_{k_y} e^{ik_x y} + F_{k_y} e^{-ik_y y}\right) \\ &\times \left(C_{k_z} e^{ik_x z} + D_{k_z} e^{-ik_y z}\right)\left(A_{k_x,k_y,k_z} e^{ic\sqrt{k_x^2+k_y^2+k_x^2}\,t} + B_{k_x,k_y,k_z} e^{-ic\sqrt{k_x^2+k_y^2+k_x^2}\,t}\right) \end{aligned}. \tag{14}$$

In this equation none of the parameters k_x, k_y, or k_z are specified.

Some general remarks concerning Eqs. (12) – (14) are in order. First, notice that all three solutions depend upon three parameters, which are (essentially) the three independent separation constants that arise in the separation-of-variables process. Second, the discrete parameters (l,m in spherical coordinates, n in cylindrical coordinates) are discrete because of mathematical considerations related to the coordinate system being used. The other parameters (k in spherical coordinates, k,a

[2] You have seen an almost general form for Cartesian coordinates in Exercise 19.2.

in cylindrical coordinates, k_x, k_y, k_z in Cartesian coordinates) can take on any values and the solutions will still satisfy the wave equation.

For a given problem, the physics of the situation may dictate that these parameters take on only certain values. For example, in Exercise 19.2, where you found the normal-mode standing waves in a rectangular room, you found that because of the boundary conditions the parameters k_x, k_y, and k_z could only take on the values

$$k_x = \frac{n_x \pi}{L_x}, \qquad k_y = \frac{n_y \pi}{L_y}, \qquad k_z = \frac{n_z \pi}{L_z}, \tag{15a) – (15c)}$$

where the n_i's are integers and the L_i's are the dimensions of the room. Physical considerations, such as boundary conditions, may also place constraints on the multiplicative factors that appear in Eqs. (12) – (14).

III. A Vibrating Circular Drumhead

Let's look at another example where physics constrains some of these unspecified parameters. In particular, let's find the normal modes of vibration of a circular drumhead. First, we must recognize that this is a two dimensional, rather than a three dimensional problem. If we were working in Cartesian coordinates we would only need *x* and y, but because we are interested in a circular drumhead we should recognize that it might be better to work in polar coordinates (with the origin at the center of the drum head). Well, if we were to write the 2D wave equation in polar coordinates and do separation of variables, the solutions would be the same as the $k^2 = a^2$ solutions for cylindrical coordinates in Eq. (13). That is, the solutions would be

$$q_{n,a}(\rho,\phi,t) = \left[G_{n,a} J_n(a\rho) + H_{n,a} Y_n(a\rho)\right]\left(E_n e^{in\phi} + F_n e^{-in\phi}\right)\left(A_a e^{iact} + B_a e^{-iact}\right). \tag{16}$$

Let's now apply some physics. First we know that we want the displacement q to be everywhere finite. So because the functions $Y_n(s)$ diverge for $s \to 0$ we must have $H_{n,a} = 0$. Also, we want the displacement to be a real quantity. With that in mind we explicitly write the ϕ and t parts of Eq. (16) in terms of sine and cosine functions, rather then the complex exponential functions.[3] We then have

$$q_{n,a}(\rho,\phi,t) = G_{n,a} J_n(a\rho)\left[\tilde{E}_n \cos(n\phi) + \tilde{F}_n \sin(n\phi)\right]\left[\tilde{A}_a \cos(act) + \tilde{B}_a \sin(act)\right], \tag{17}$$

[3] There are, of course, other ways to make sure that the solution is real. See the discussion on p. 8 of the Lecture 2 notes.

where the quantities with tildes in Eq. (17) are real multiplicative factors [that can be related to the quantities without tildes in Eq. (16), if necessary].

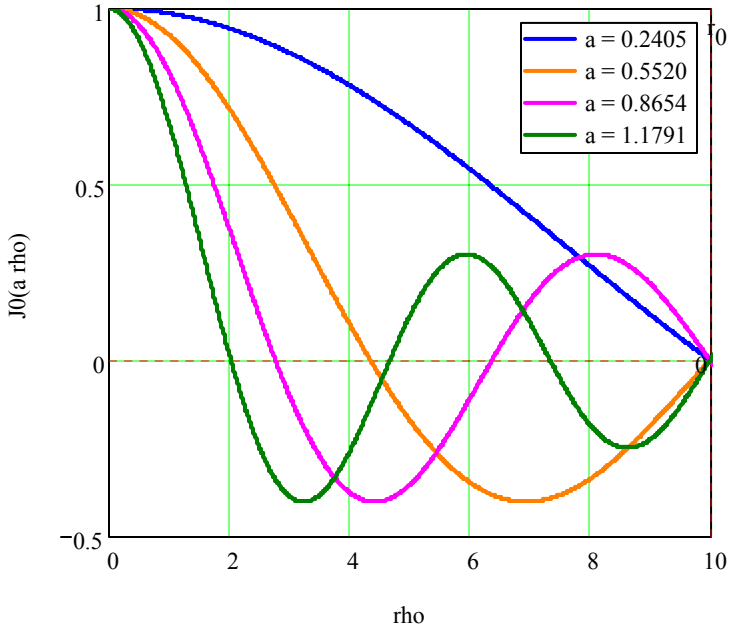
There is now one more bit of physics to consider: the boundary condition at the edge of the drum head. For simplicity, we assume that this bc is $q_{n,a}(\rho_0,\phi,t)=0$, where ρ_0, is the radius of the drumhead. Applying this bc to Eq. (17) then gives us

$$0 = G_{n,a}J_n(a\rho_0)\left[\tilde{E}_n\cos(n\phi)+\tilde{F}_n\sin(n\phi)\right]\left[\tilde{A}_a\cos(act)+\tilde{B}_a\sin(act)\right]. \tag{18}$$

So how can Eq. (18) be satisfied? The only nontrivial way is to require that a be such that $J_n(a\rho_0)=0$. Now, each Bessel function J_n has an infinite number of discrete zeros (see the figure on p. 5 of Lecture 27 notes) so that there are an infinite number of discrete values of a (which are different for each n) that will satisfy Eq. (18). Unfortunately, in contrast to the Cartesian coordinate example specified by Eq. (15), there are no nice, simple formulae for the zeros of the Bessel functions. Nonetheless, the zeros can be found numerically.

A. $n=0$ Normal Modes

We first look at normal mode solutions specified by $n=0$. For these solutions the Bessel function $J_0(s)$ comes into play. The zeros of this function are equal to 2.405, 5.520, 8.654, 11.791, …[4] Thus, the bc will be satisfied for



[4] The zeros are tabulated in *Handbook of Mathematical Functions* by Abramowitz and Stegun (where else?).

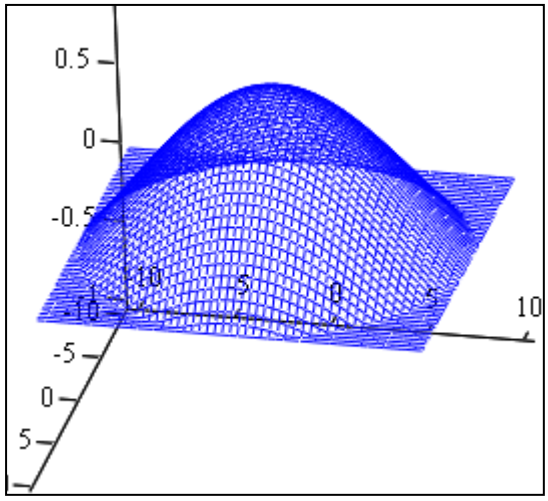
$$a\rho_0 = 2.405,\ 5.520,\ 8.654,\ 11.791,\ \ldots \tag{20}$$

This is illustrated in the graph on the previous page, where we have set $\rho_0 = 10$. Notice that $J_0(a\rho)$ is indeed equal to zero at $\rho = \rho_0$ for each value of a given by Eq. (20).

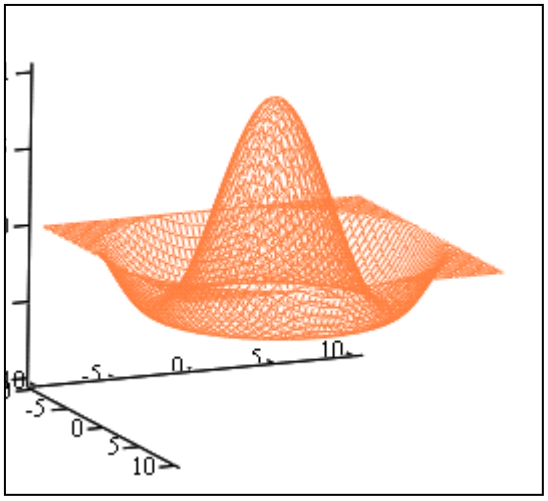
Let's now look at the complete solution for $n = 0$. Simplifying Eq. (17) we can write the $n = 0$ normal modes as

$$q_{0,i}(\rho,\phi,t) = G_{0i} J_0(a_{0i}\rho)\,\widetilde{E}_0\left[\widetilde{A}_{0i}\cos(a_{0i}ct) + \widetilde{B}_{0i}\sin(a_{0i}ct)\right], \tag{21}$$

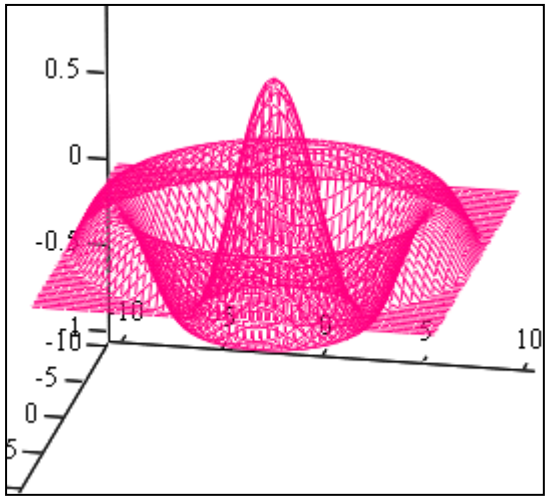
where $a_{0i}\rho_0$ is the i'th zero of $J_0(s)$. Notice that in Eq. (21) we have changed the labeling of the solution; we now label the normal modes with two integers: the first



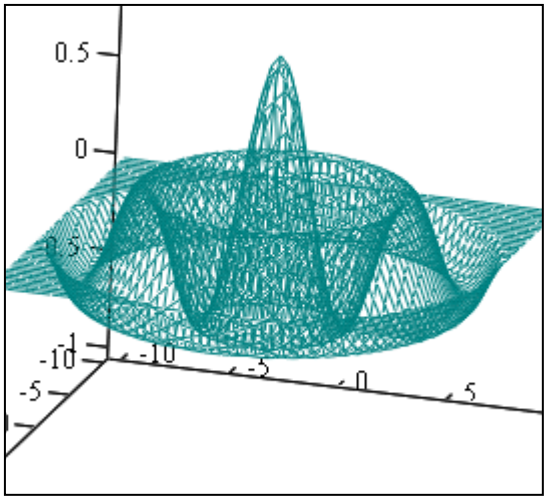
z1



z2



z3



z4

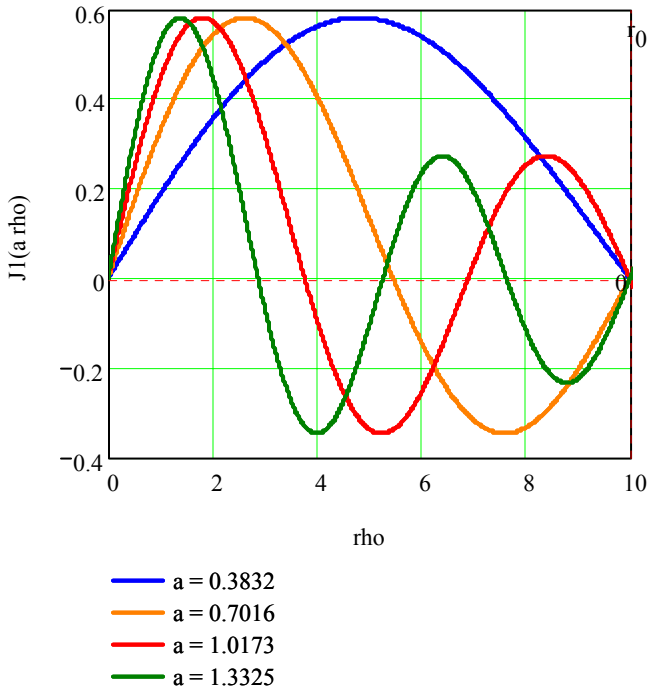
$(=0)$ corresponds to n, and the second (i) labels the value of a that makes the solution vanish at the boundary. Notice that the only spatial variable in Eq. (21) is ρ: the dependence on ϕ is gone. Snapshots of first four normal-mode solutions are shown on the previous page. The class web site has animated (time dependent) versions of these solutions. As evident in the animations [and should be evident from Eq. (21)], these solutions are radially symmetric versions of standing waves.

B. $n=1$ *Normal Modes*

For any other value of n, the normal modes are found in essentially the same manner. We must again satisfy the bc at the edge of the drum head, which determines the values of a. For $n=1$ the zeros of $J_1(s)$ are 3.832, 7.016, 10.173, 13.325, … Thus, for $n=1$ the boundary condition is satisfied for

$$a\rho_0 = 3.832,\ 7.016,\ 10.175,\ 13.325,\ \ldots \tag{22}$$

This is illustrated in the following figure.



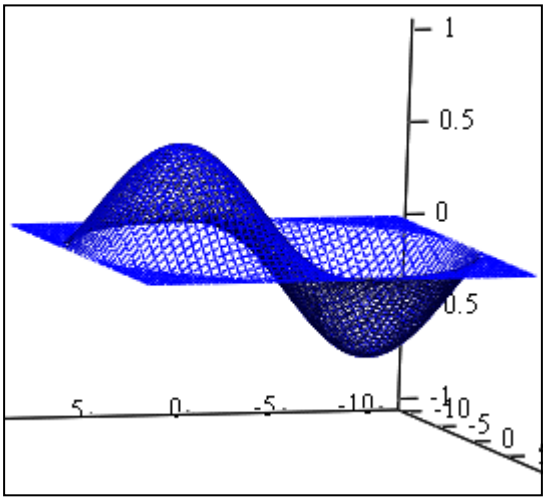
For the complete solution we thus have

$$q_{1,i}(\rho,\phi,t) = G_{1i}J_1(a_{1i}\rho)\left[\widetilde{E}_1\cos(\phi)+\widetilde{F}_1\sin(\phi)\right]\left[\widetilde{A}_{1i}\cos(a_{1i}ct)+\widetilde{B}_{1i}\sin(a_{1i}ct)\right]. \tag{23}$$

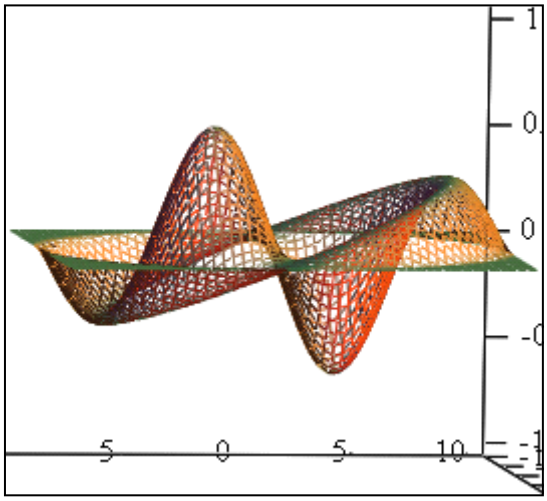
Because the ϕ dependence is no longer trivial, this solution is a bit more complicated than that for $n=0$. For $n=0$ the disappearance of ϕ resulted in only one linearly independent solution (in terms of spatial variables – there are still two linearly independent solutions if one considers time). Here, however, the $\cos(\phi)$ and $\sin(\phi)$ solutions are linearly independent. For simplicity, let's just consider the solution with $\widetilde{F}_1 = 0$, which leaves only the $\cos(\phi)$ term. Then we have

$$q_{1,i}(\rho,\phi,t) = G_{1,i} J_1(a_{1i}\rho)\,\widetilde{E}_1 \cos(\phi)\left[\widetilde{A}_i \cos(a_{1i}ct) + \widetilde{B}_i \sin(a_{1i}ct)\right] . \tag{24}$$

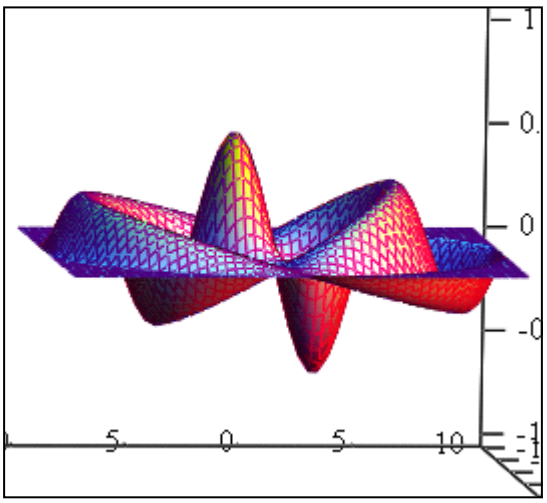
The following figure shows snapshots of this solution. Animated versions are again available on the class web site.



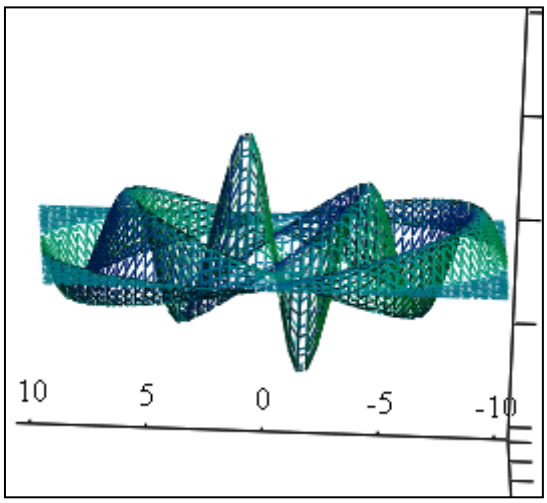
z1



z2



z3



z4

IV. Concluding Remarks

That is it for separation of variables (until you run into them again in some later course, or perhaps while doing some research!). Summarizing, we have seen that we can obtain solutions to the wave equation in three different coordinate systems using this technique. Sometimes these solutions are simple, sometime they are not so simple, at least in terms of functions with which you may be familiar. Each solution is labeled by three independent separation constants, which may or may not be constrained to certain values. Because the ordinary differential equations that give us these solutions are homogeneous and linear, there are also undetermined multiplicative factors associated with each part of the solution. Often (at least) some of the separation constants and the multiplicative factors are determined by physical considerations, such as imposed boundary conditions. In the example that we just did we saw that the parameter a must take on discrete values in order for the boundary condition at the edge of the drumhead to be satisfied.

While separation-of-variables solutions can be interesting in their own right (as in the case of the drumhead modes), I'll again remind you that they are also quite useful because they can be used to construct a basis for any solution to the wave equation, much as we previously discussed for the 1D wave equation. This point has been previously discussed in Sec. III of the Lecture 19 notes.

Exercises

*__23.1__ Using the definition of s and the chain rule, derive Eq. (7) from Eq. (6). (Hint: you may wish to review the Lecture 21 notes.)

*__23.2__ The figure on p. 2 indicates that $j_2(0)=0$. Using Eq. (10e) show that this is indeed the case.

*__23.3__ The two linearly independent combinations of the spherical Bessel functions

$$h_l^{(1)}(s)=j_l(s)+iy_l(s) \text{ and } h_l^{(2)}(s)=j_l(s)-iy_l(s)$$

are know as spherical Bessel functions of the *third kind*. Using these definitions and Eq. (10), express $h_1^{(1)}(s)$ and $h_1^{(2)}(s)$ in terms of the functions e^{is} and e^{-is}.

*__23.4 Normal Modes Inside a Sphere__.
Starting with Eq. (12) find all normal-mode solutions to the wave equation inside a sphere that satisfy **all** of the following conditions: the solutions are (1) real, (2) spherically symmetric, (3) finite everywhere, and (4) vanish on the boundary of the sphere, which has a radius of r_0.

Energy Density / Energy Flux / Total Energy in 1D

Overview and Motivation: From your study of waves in introductory physics you should be aware that waves can transport energy from one place to another – consider the generation and detection of radio waves, for example. In the next two lectures we consider some of the details of the energy associated with wave phenomena. To keep it initially simple, we start out with one dimensional waves. In the next lecture we generalize the concepts discussed here to three dimensions.

Key Mathematics: density, flux, and the continuity equation.

I. Density, Flux, and the Continuity Equation

Let's start by considering some quantity Q that has associated with it a density ρ. Because we are interested in only one (spatial) dimension, the density associated with Q will be so much Q per unit length. If we then integrate that density between two points in space, x_1 and x_2, then we will get the total amount of Q between the points x_1 and x_2. Mathematically, we write this as

$$Q(x_1, x_2, t) = \int_{x_1}^{x_2} \rho(x,t)\, dx \tag{1}$$

We have explicitly included time because Q may be a dynamic quantity.

Often, Q is a conserved quantity. That is, it cannot be either created or destroyed. If that is the case then the change in Q within the region from x_1 to x_2

$$\frac{\partial Q(x_1, x_2, t)}{\partial t} = \int_{x_1}^{x_2} \frac{\partial \rho(x,t)}{\partial t}\, dx \tag{2}$$

must be equal to the net flow of Q into the region. That is,

$$\frac{\partial Q(x_1, x_2, t)}{\partial t} = j(x_1, t) - j(x_2 t), \tag{3}$$

where j is the Q **current density** (or **flux**). Convention is that if $j > 0$, then the flow is in the positive x direction, and if $j < 0$, then the flow is the negative x direction. Note that the units of ρ are $[Q]$/m and the units of j are $[\mathrm{Q}]/\mathrm{s} = [\rho]\mathrm{m/s}$. For example, if Q represents charge, then $[\rho]$ = Coulomb/m and $[j]$ = Coulomb/s.

If we now equate the rhs's of Eqs. (2) and (3) we get

$$\int_{x_1}^{x_2} \frac{\partial \rho(x,t)}{\partial t}\, dx = j(x_1,t) - j(x_2 t). \tag{4}$$

Now the rhs of Eq. (4) can be written as

$$j(x_1,t) - j(x_2 t) = -\int_{x_1}^{x_2} \frac{\partial j(x,t)}{\partial x}\, dx \tag{5}$$

and so we can rewrite Eq. (4) as

$$\int_{x_1}^{x_2} \left[\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} \right] dx = 0. \tag{6}$$

Now, because the limits x_1 and x_2 are arbitrary, the integrand must vanish. This gives us an important relationship between the density and flux,

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0. \tag{7}$$

Equation (7) is known as the (1D) **continuity equation**. Because the density and flux are *local* quantities (which means that they can be defined at each point in space, as opposed to Q, which is a *global* quantity), Eq. (7) is a local statement about the conservation of Q.

II. Energy Density and Flux for 1D Waves

Let's now apply this discussion to the energy associated with 1D waves. That is, we let Q be the total energy associated with 1D waves between two points x_1 and x_2. To be specific, let's think about transverse waves on a string. For this particular physical system, where the wave speed c is given by $c = \sqrt{\tau/\mu}$, where τ is the tension in the string and μ is the mass density (mass per unit length), the energy density can be written as[1]

[1] We do not prove this result here. For its derivation we refer you to an intermediate mechanics text, such *Classical Dynamics* by Marion and Thornton.

$$\rho(x,t)=\frac{\mu}{2}\left(\frac{\partial q}{\partial t}\right)^2+\frac{\tau}{2}\left(\frac{\partial q}{\partial x}\right)^2 \tag{8}$$

The first term on the rhs is the **kinetic energy density** ρ_T while the second is the **potential energy density** ρ_V.

So, we have the energy density, but what about the energy flux j? Well, whatever it is it must satisfy Eq. (7), the continuity equation. Let's thus calculate $\partial\rho/\partial t$ and see what happens. Using Eq. (8) we have

$$\frac{\partial\rho}{\partial t}-\left[\mu\frac{\partial q}{\partial t}\frac{\partial^2 q}{\partial t^2}+\tau\frac{\partial q}{\partial x}\frac{\partial^2 q}{\partial t\partial x}\right]=0 \tag{9}$$

Comparing this with Eq. (7) we see that we would like to be able to write

$$-\left[\mu\frac{\partial q}{\partial t}\frac{\partial^2 q}{\partial t^2}+\tau\frac{\partial q}{\partial x}\frac{\partial^2 q}{\partial t\partial x}\right] \tag{10}$$

as $\partial/\partial x$ of some quantity, which we could then identify as the flux j. To do this we can get some help from the wave equation (here we use $c^2=\tau/\mu$ for string waves),

$$\frac{\partial^2 q}{\partial t^2}=\frac{\tau}{\mu}\frac{\partial^2 q}{\partial x^2}, \tag{11}$$

and the equality of mixed partial derivatives,

$$\frac{\partial}{\partial t}\left(\frac{\partial q}{\partial x}\right)=\frac{\partial}{\partial x}\left(\frac{\partial q}{\partial t}\right), \tag{12}$$

to rewrite Eq. (9) as

$$\frac{\partial\rho}{\partial t}-\tau\left[\frac{\partial q}{\partial t}\frac{\partial^2 q}{\partial x^2}+\frac{\partial q}{\partial x}\frac{\partial^2 q}{\partial x\partial t}\right]=0, \tag{13}$$

which can be compacted as

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}\left\{-\tau\frac{\partial q}{\partial t}\frac{\partial q}{\partial x}\right\}=0. \tag{14}$$

We can thus identify the energy flux as

$$j(x,t) = -\tau \frac{\partial q}{\partial t}\frac{\partial q}{\partial x}. \tag{15}$$

III. Several Examples

Let's look at three examples: a traveling wave, a standing wave, and two colliding wave packets. In each example we consider the two energy densities ρ_T and ρ_V and the energy flux j.

A. Traveling Wave

To follow along at this point you will need to go to the class web site and bring up the video file *Energy in 1D Traveling Wave.avi*, which shows these time dependent quantities for the traveling wave

$$q(x,t) = q_0 \cos(kx - ckt). \tag{16}$$

Notice that, as perhaps expected, that all quantities move to the right at the wave speed c. Furthermore, the "wavelength" of the energy densities and flux is half that of the displacement q. For the energy densities, this should be obvious from their definitions. Furthermore, because for this traveling-wave example it is not hard to show that $j = c\rho$, j looks essentially the same as the total energy density ρ.

B. Standing Wave

The next video on the web site, *Energy in 1D Standing Wave.avi*, shows these same time dependent quantities for the standing wave

$$q(x,t) = q_0 \sin(kx)\cos(ckt). \tag{17}$$

This example is a bit more interesting. Notice that now the energy oscillates back and forth between kinetic and potential, which now have their (stationary) maxima at different spatial points. A careful examination of the flux shows that the energy at a given point flows one direction and then the other as it is converted between potential and kinetic.

C. Colliding wave packets

The last example can be found in the video *Energy in 1D Colliding Pulses.avi*. The displacement for this wave is given by

$$q(x,t) = q_0 \cos(kx - ckt)\, e^{-[(kx-ckt)/a_0]^2} - \left[q_0 \cos(kx + ckt)\, e^{-[(kx+ckt)/a_0]^2} \right]. \tag{18}$$

For most of the time the wave looks like two noninteracting wave packets (or pulses), each moving at the speed c but in different directions. Notice that when the pulses are far apart the behavior of the density and flux is similar to that for a traveling wave, but as the pulses overlap the density and flux behave in a manner similar to a standing wave (which can, of course, be described as the superposition of two traveling waves).

IV. Total Energy

Now that we have seen some examples illustrating the local quantities $\rho(x,t)$ and $j(x,t)$, let's consider the total energy associated with wave motion. In particular, let's consider transverse waves on a string on the interval $0 \le x \le L$ with the standard boundary conditions $q(0,t) = q(L,t) = 0$. In that case we can write any wave on the string as a linear superposition of standing waves as[2]

$$q(x,t) = \sum_{n=1}^{\infty} \sin\left(\tfrac{n\pi}{L} x\right) \left[A_n \cos(\omega_n t) + B_n \sin(\omega_n t) \right], \tag{19}$$

where $\omega_n = n\pi c/L$, and the coefficients A_n and B_n depend upon the initial conditions.

Using Eq. (1) the total kinetic and potential energies can be expressed in terms of their densities as

$$T(t) = \int_0^L \rho_T(x,t)\, dx = \frac{\mu}{2} \int_0^L \left(\frac{\partial q}{\partial t} \right)^2 dx, \tag{20a}$$

$$V(t) = \int_0^L \rho_V(x,t)\, dx = \frac{\tau}{2} \int_0^L \left(\frac{\partial q}{\partial x} \right)^2 dx, \tag{20b}$$

Let's now substitute the general form of the displacement on the rhs of in Eq. (19) into Eq. (20) and calculate the total kinetic and potential energies. For the kinetic energy we have

[2] See Lecture 10 notes.

$$T(t)=\frac{\mu}{2}\int_0^L\left\{\sum_{n=1}^{\infty}\sin\left(\tfrac{n\pi}{L}x\right)\omega_n\left[-A_n\sin(\omega_n t)+B_n\cos(\omega_n t)\right]\right\}\times\left\{\sum_{m=1}^{\infty}\sin\left(\tfrac{m\pi}{L}x\right)\omega_m\left[-A_m\sin(\omega_m t)+B_m\cos(\omega_m t)\right]\right\}dx \tag{21}$$

Notice that we use different indices on the two sums so that we know which quantities go with each sum. Switching the orders of integration and summation we can rewrite Eq. (21) as

$$T(t)=\frac{\mu}{2}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left\{\omega_n\omega_m\left[-A_n\sin(\omega_n t)+B_n\cos(\omega_n t)\right]\left[-A_m\sin(\omega_m t)+B_m\cos(\omega_m t)\right]\times\int_0^L\sin\left(\tfrac{n\pi}{L}x\right)\sin\left(\tfrac{m\pi}{L}x\right)dx\right\} \tag{22}$$

We can now simplify this considerably because of the orthogonality of the sine functions. That is, using

$$\int_0^L\sin\left(\tfrac{n\pi}{L}x\right)\sin\left(\tfrac{m\pi}{L}x\right)dx\Big\}=\frac{L}{2}\delta_{nm}, \tag{23}$$

Eq. (22) becomes

$$T(t)=\frac{\mu L}{4}\sum_{n=1}^{\infty}\omega_n^2\left[A_n\sin(\omega_n t)-B_n\cos(\omega_n t)\right]^2. \tag{24}$$

Now

$$T_n(t)=\frac{\mu L}{4}\omega_n^2\left[A_n\sin(\omega_n t)-B_n\cos(\omega_n t)\right]^2 \tag{25}$$

is simply the kinetic energy contained in the n th normal mode. Thus Eq. (24) can be simply viewed as the sum of kinetic energies contained in all of the normal modes,

$$T(t)=\sum_{n=1}^{\infty}T_n(t) \tag{26}$$

Similarly, starting with Eq. (20b), one can show that the total potential energy can be written as

$$V(t)=\sum_{n=1}^{\infty}V_n(t), \tag{27}$$

where

$$V_n(t)=\frac{\mu L}{4}\omega_n^2\left[A_n\cos(\omega_n t)+B_n\sin(\omega_n t)\right]^2 \tag{28}$$

is the potential energy contained in each normal mode. Further, using Eqs. (25) and (28) it is not difficult to show that the total energy contained in each mode, $E_n(t)=T_n(t)+V_n(t)$, is equal to

$$E_n(t)=\frac{\mu L}{4}\omega_n^2\left(A_n^2+B_n^2\right), \tag{29}$$

and is thus constant. That the energy in each normal mode is constant is due to the fact that the normal modes do not interact. Why? Because the equation of motion for each normal mode is independent of the other normal modes. Notice also that the energy is each normal mode is proportional the square of the amplitude $\left(A_n^2+B_n^2\right)$. Finally, because $E_n(t)$ is constant, the total energy

$$E(t)=\sum_{n=1}^{\infty}E_n(t) \tag{30}$$

is also constant.

Exercises

*__24.1__. **Energy Density and Current for a Traveling Wave**. Consider the traveling wave solution to the 1D wave equation $q(x,t) = q_0 \cos(kx - ckt)$.
(**a**) Calculate the kinetic, potential and total energy densities $\rho_T(x,t)$, $\rho_V(x,t)$, and $\rho(x,t)$, respectively, and the energy current density $j(x,t)$. Show that $\rho_T(x,t) = \rho_V(x,t)$. Further show that $j(x,t) = c\rho(x,t)$.
(**b**) Does the energy current flow in the direction that you expect? Explain.
(**c**) Show that the 1D continuity equation is satisfied by your expressions for $\rho(x,t)$ and $j(x,t)$.

__24.2__. **Energy Density and Current for a Standing Wave. Consider the standing-wave solution to the wave equation for transverse waves on a string $q(x,t) = q_0 \sin(kx)\sin(\omega t)$.
(**a**) Calculate the kinetic and potential energy densities $\rho_T(x,t)$ and $\rho_V(x,t)$, respectively, and the energy current density $j(x,t)$. Express your answers using the parameters μ, c, and ω.
(**b**) Show that the 1D continuity equation [Eq. (7)] is satisfied for this wave.
(**c**) For this wave find the total kinetic energy $T(t)$ and potential energy $V(t)$ in a string of length L on the interval $0 \le x \le L$, assuming that $k = n\pi/L$, where n is some positive integer. Here, use the parameters μ, L, and ω to express your answers.
(**d**) Show that the total energy $E(t) = T(t) + V(t)$ is independent of time.

*__24.3 Total Energy in Vibrating String__.
(**a**) As was done for the kinetic energy in Sec. IV, show that the total potential energy contained in the vibrating string is given by

$$V(t) = \frac{\mu L}{4} \sum_{n=1}^{\infty} \omega_n^2 \left[A_n \cos(\omega_n t) + B_n \sin(\omega_n t)\right]^2$$

(**b**) Using Eqs. (25) and (28) show that the total energy $E_n(t)$ in a normal mode is constant.

*__24.4__ Consider the generic traveling wave $q(x,t) = f(x - ct)$. Show that for this wave
(**a**) $\rho_T = \rho_V$ and
(**b**) $j = c\rho$.

Energy Density / Energy Flux / Total Energy in 3D

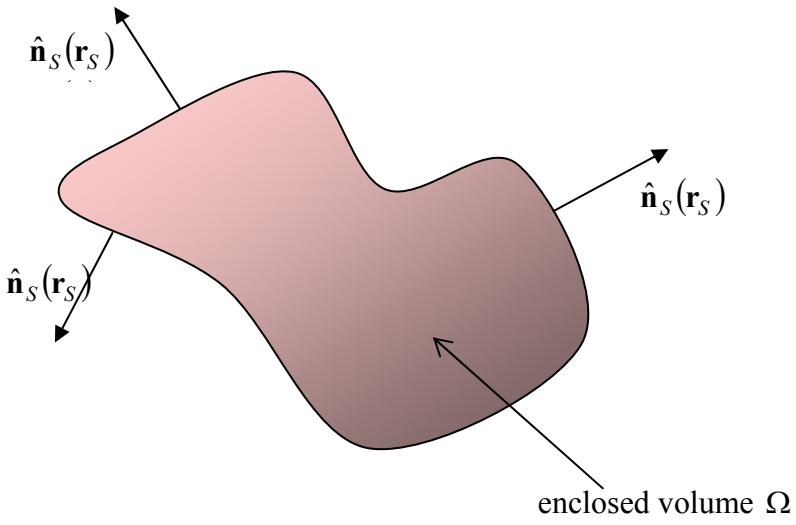
Overview and Motivation: In this lecture we extend the discussion of the energy associated with wave motion to waves described by the 3D wave equation. In fact, the first part of the discussion is exactly the same as the 1D case, just extended to 3D. In the examples we look at the energy associated with spherically symmetric waves.

Key Mathematics: Some 3D calculus, especially the divergence theorem and the spherical-coordinates version of the gradient.

I. Density, Flux, and the Continuity Equation

As in the 1D case let's assume that we are interested in some quantity $Q(t)$ that has an associated density $\rho(x,t)$. Since we are dealing with a density that lives in a 3D space, the units of density will be the units of Q divided by m^3. That is, $[\rho]=[Q]/\text{m}^3$.

Let's consider a volume Ω enclosed by a surface S, as illustrated in the following figure. At each point on the surface we define a perpendicular, outward-pointing unit vector $\hat{\mathbf{n}}_S(\mathbf{r}_S)$ associated with each point $\mathbf{r}_S$ on the surface.



The amount of Q contained in Ω can be written as

$$Q_\Omega(t)=\int_\Omega \rho(\mathbf{r},t)\,d^3r \tag{1}$$

As in the 1D case, if Q is a conserved quantity, then the change in Q inside Ω,

$$\frac{dQ_\Omega(t)}{dt} = \int_\Omega \frac{\partial \rho(\mathbf{r},t)}{\partial t}\, d^3r\,, \tag{2}$$

must be equal to the net flow of Q into Ω,

$$\frac{dQ_\Omega(t)}{dt} = -\oint_S \mathbf{j}(\mathbf{r}_S,t)\cdot \hat{n}_S(\mathbf{r}_S)\, dS\,. \tag{3}$$

The (vector) quantity $\mathbf{j}$ is again known as the Q **current density** or the Q **flux**. The dimensions of $\mathbf{j}$ are the dimensions of ρ times a velocity, so $[\mathbf{j}] = [\rho]\text{m/s}$. Thus also $[\mathbf{j}] = [Q]/(\text{m}^2\text{s})$. Note that the rhs of Eq. (3) can be interpreted as the **total** Q **current** flowing out through the surface S. Equating the rhs's of Eqs. (2) and (3) gives us

$$\int_\Omega \frac{\partial \rho(\mathbf{r},t)}{\partial t}\, d^3r = -\oint_S \mathbf{j}(\mathbf{r}_S,t)\cdot \hat{\mathbf{n}}_S(\mathbf{r})\, dS\,. \tag{4}$$

We can now use the **divergence theorem** (which is one of several 3D extensions of the fundamental theorem of calculus),

$$\int_\Omega \nabla\cdot \mathbf{A}(\mathbf{r}_S)\, d^3r = \oint_S \mathbf{A}(\mathbf{r})\cdot \hat{\mathbf{n}}_S(\mathbf{r}_S)\, dS\,, \tag{5}$$

to rewrite Eq. (4) as

$$\int_\Omega \left[\frac{\partial \rho(\mathbf{r},t)}{\partial t} + \nabla\cdot \mathbf{j}(\mathbf{r},t)\right] d^3r = 0 \tag{6}$$

Now, because the volume Ω is arbitrary, the integrand must vanish. Thus

$$\frac{\partial \rho(\mathbf{r},t)}{\partial t} + \nabla\cdot \mathbf{j}(\mathbf{r},t) = 0\,. \tag{7}$$

Equation (7) is the 3D version of the **continuity equation**, which again is a local statement of the conservation of Q.

II. Energy Density and Flux for 3D Waves

We now apply this discussion to the energy associated with 3D waves. In this case Q represents the energy associated with a wave (within some volume). For waves described by the 3D wave equation the energy density can be written as

$$\rho(\mathbf{r},t)=\frac{\mu}{2}\left[\left(\frac{\partial q}{\partial t}\right)^2+c^2(\nabla q)^2\right], \tag{8}$$

where $q(\mathbf{r},t)$ is the variable that is governed by the wave equation. The first term on the rhs of Eq. (8) is the kinetic energy density ρ_T, and the second is the potential energy density ρ_V. Now Eq. (8) is fairly general as long as μ is suitably interpreted. If q is a true displacement, then μ will be a parameter with the units of mass density. If q represents something else, say an electric field, then it will have some other units. From Eq. (8) it is fairly easy to see that the units of μ are generally given by $[\mu]=(\text{Joule s}^2)/(\text{m}^3\ [q]^2)$. It is not hard to show that the energy flux, which can be written as

$$\mathbf{j}(\mathbf{r},t)=-\mu c^2\frac{\partial q}{\partial t}\nabla q\,, \tag{9}$$

together with the energy density in Eq. (8) satisfy Eq. (7), the continuity equation.

III. Several Examples

Let's look at some examples that involve spherically symmetric waves.

A. Spherical Standing Wave

Let's look at a standing-wave example. You may recall that a spherical-coordinates separable solution that is finite everywhere is of the form

$$q_{k,l,m}(r,\theta,\phi,t)=C_{k,l,m}\ j_l(kr)\,P_l^m(\cos(\theta))\left(C_m e^{im\phi}+D_m e^{-im\phi}\right)\left(A_k e^{ikct}+B_k e^{-ikct}\right), \tag{10}$$

where j_l is a spherical Bessel function (of the first kind), and P_l^m is an associated Legendre function (of the first kind). The parameter m is an integer whose absolute value can be no larger than the nonnegative integer l. If we want a solution with spherical symmetry, then there can be no θ or ϕ dependence. This means that both l and m must be zero because the only associated Legendre function independent of θ is $P_0^0(\cos(\theta))=1$. Thus, the spherical Bessel function in Eq. (10) must be $j_0(kr)=\sin(kr)/(kr)$, and so Eq. (10) simplifies to

$$q_{k,0,0}(r,\theta,\phi,t) = C_{k,0,0}\,\frac{\sin(kr)}{kr}\left(A_k e^{ikct} + B_k e^{-ikct}\right). \tag{11}$$

If we simplify this further by letting A_k be a real number and let $B_k = A_k$ (making the solution explicitly real) then we have

$$q_{k,0,0}(r,\theta,\phi,t) = 2A_k C_{k,0,0}\,\frac{\sin(kr)}{kr}\cos(kct). \tag{12}$$

Because all parts of the system oscillate with the same phase, this is a spherically symmetric version of a standing wave.

Using Eqs. (8) and (9) we can calculate the kinetic and potential energy densities and the energy flux associated with the wave in Eq. (12). To do this in a fairly simple manner we can use the spherical-coordinates version of the gradient

$$\nabla f(r,\theta,\phi) = \frac{\partial f}{\partial r}\hat{\mathbf{r}} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{r\sin(\theta)}\frac{\partial f}{\partial \phi}\hat{\boldsymbol{\varphi}}, \tag{13}$$

where $\hat{\mathbf{r}}$, $\hat{\boldsymbol{\theta}}$, and $\hat{\boldsymbol{\varphi}}$ are unit vectors in the r, θ, and ϕ directions, respectively. The nice thing about spherically symmetric solutions is that only the first term on the rhs of Eq. (13) contributes to the gradient.

A video of q, ρ_T, ρ_V, and j for the wave in Eq. (12), *Energy in 3D Standing Wave.avi*, is available on the class web site. As the video shows, the displacement is indeed a standing wave. Unfortunately, the energy densities and flux fall off with the radial distance r so fast that it is hard to really see their behavior.

Given this, we have made another video, *Energy in 3D Standing Wave 2.avi*, which plots the surface integrated density and flux,[1]

$$D(r) = \oint_S \rho(\mathbf{r}_S)\,dS, \tag{14}$$

and

$$I(r) = \oint_S \mathbf{j}(\mathbf{r})\cdot\hat{\mathbf{n}}_S(\mathbf{r}_S)\,dS, \tag{15}$$

[1] The video separately shows the kinetic and potential contributions to $D(r)$.

where the surface S is of radius r centered at the origin. Now because a spherically symmetric solution is independent of the two angles θ and ϕ, this amounts to multiplying the density ρ and flux $\mathbf{j}$ by the factor $4\pi r^2$, which is the surface area of the sphere S. The quantity $D(r)$ (which has units of Joule/m) can be though of as a linear energy density (i.e., the energy per unit length along the radial direction), while the quantity $I(r)$ (which has units of Joule/s) is the total (energy) current flowing through S. Notice that this new video is very similar to the 1D standing wave video that we looked at in the last lecture.

B. Spherical Traveling Wave

Let's also look at a spherically symmetric traveling wave. If we are thinking about sound waves, this is the sort of wave that would result from a pulsating sphere centered at the origin. We can construct a traveling wave solution from a linear combination of 2 linearly independent standing waves. We thus need to use both kinds of spherical Bessel functions. The linear combination that produces a spherically symmetric, outgoing, traveling wave is[2]

$$q_{k,0,0}(r,\theta,\phi,t) = C_{k,0,0}\left[j_0(kr)\cos(kct) - y_0(kr)\sin(kct)\right]. \tag{16}$$

which can be written in terms of sine and cosine functions as

$$q_{k,0,0}(r,\theta,\phi,t) = C_{k,0,0}\left[\frac{\sin(kr)}{kr}\cos(kct) - \frac{\cos(kr)}{kr}\sin(kct)\right]. \tag{17}$$

The video, *Energy in 3D Traveling Wave.avi*, shows $D(r)$ and $I(r)$ for this wave. Indeed, away from the origin the wave appears to be an outgoing traveling wave. However, at the origin something rather different seems to be happening – something with some standing-wave character, perhaps?

Well, as it turns out, the current density $\mathbf{j}$ has terms with two types of behavior. The first type has a $1/r^2$ dependence. These terms describe the **radiative** part of the wave, which carries energy off to infinity. Because the radiative part of $\mathbf{j}$ varies as $1/r^2$ the radiative part of $I(r)$ does not vanish as $r \to \infty$. However, there are also **nonradiative** terms, which vary as $1/r^3$. These terms act more like a standing wave: the energy associated with these terms just oscillates back and forth and never really goes anywhere. Because of the $1/r^3$ behavior to the nonradiative part of $\mathbf{j}$, the current $I(r)$ associated with these terms vanishes as $1/r$ as $r \to \infty$. These terms are

[2] Note that this solution is only valid in the region of space outside the source. In the video you may think of the source as being infinitesimally small, so that the solution is valid infinitesimally close to the origin.

thus sometimes called the **local fields** associated with the source. In the video *Energy in 3D Traveling Wave 2.avi* we separately show the current $I(r)$ associated with each type of term. Notice that the radiative piece looks essentially like a 1D traveling wave while the nonradiative piece is really only important in the vicinity of the origin.

Exercises

*__25.1__ Show that the expressions for the density ρ and $\mathbf{j}$ in Eqs. (8) and (9), respectively, satisfy Eq. (7), the continuity equation.

**__25.2 Spherical Traveling Wave__
(**a**) Write the wave in Eq. (17),

$$q_{k,0,0}(r,\theta,\phi,t) = C_{k,0,0}\left[\frac{\sin(kr)}{kr}\cos(kct) - \frac{\cos(kr)}{kr}\sin(kct)\right],$$

as an explicit function of $(r-ct)$, thus showing that it is a traveling wave moving outward from the origin.
(**b**) Using your result from part (a), show that the radiative and nonradiative components of the current density $\mathbf{j}$ can be written, respectively, as

$$\mathbf{j}_R(r,t) = \frac{\mu c^3 q_0^2}{r^2}\cos^2(kr-kct)\,\hat{\mathbf{r}} \quad \text{and} \quad \mathbf{j}_{NR}(r,t) = -\frac{\mu c^3 q_0^2}{kr^3}\cos(kr-kct)\sin(kr-kct)\,\hat{\mathbf{r}}\,.$$

(**c**) Calculate the time average of each of these current-density components (defined as $\frac{1}{T}\int_0^T \mathbf{j}(r,t)\,dt$, where T is one period of oscillation) and show that the average of the radiative part points in the positive $\hat{\mathbf{r}}$ direction, while the time average of the nonradiative part is zero. (Note: neither answer should have any dependence on T.)

*__25.3 Plane Wave Energy Density__. Consider the plane-wave solution to the 3D wave equation $q(x,y,z,t) = q_0\exp\{i(k_x x + k_y y + k_z z - kct)\}$.
(**a**) Calculate the kinetic, potential, and total energy densities $\rho_T(x,y,z,t)$, $\rho_V(x,y,z,t)$, and $\rho(x,y,z,t)$, respectively and the energy current density $\mathbf{j}(x,y,z,t)$.
(**b**) Show that the 3D continuity equation is satisfied by your expressions for ρ and $\mathbf{j}$.

25.4 **Spherical Standing Wave Energy Density. Consider the spherically symmetric standing wave solution to the 3D wave equation

$q(r,\theta,\phi) = q_0 \dfrac{\sin(kr)}{kr}\cos(kct)$.

(**a**) Calculate the kinetic, potential, and total energy densities $\rho_T(r,\theta,\phi,t)$, $\rho_V(r,\theta,\phi,,t)$, and $\rho(r,\theta,\phi,,t)$, respectively.

(**b**) Show for large distances from the origin ($kr >> 1$) that the total energy density for this wave is approximately $\rho(r,\theta,\phi,,t) = \dfrac{\mu}{2} q_0^2 (kc)^2 \left\{ \left[\dfrac{\sin(kr)}{kr}\sin(kct) \right]^2 + \left[\dfrac{\cos(kr)}{kr}\cos(kct) \right]^2 \right\}$.

The 1D Schrödinger Equation for a Free Particle

Overview and Motivation: Here we look at the 1D Schrödinger equation (SE), an equation that describes the quantum motion of a nonrelativistic particle. The SE can have solutions similar to those of the wave equation (WE). In fact, as we shall see, the normal-mode solutions to the SE for a free particle (one not subject to any force) are very similar to those of the wave equation: they are traveling (or standing) waves that oscillate harmonically in space and time. An importance difference, though, is that the dispersion relation $\omega(k)$ is not the same for both equations. This leads to key differences in the general solutions that are built up from the normal-mode solutions.

Key Mathematics: We use separation of variables to find solutions to the SE. The solution to the initial-value problem will be specified in terms of the initial conditions using the Fourier transform, as we previously did for the WE (see Lecture 17).

I. The 1D Schrödinger Equation

The 1D SE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x,t)\psi=i\hbar\frac{\partial\psi}{\partial t} \tag{1}$$

is a homogeneous and linear partial differential equation for the function $\psi=\psi(x,t)$, which is often referred to as the **wave function**. While we will not worry too much about the physical significance of this equation (that will be left to a quantum-mechanics class), we point out that $\hbar=h/(2\pi)$ (where h is Planck's constant), m is the mass of the particle being described by the SE, and $V(x,t)$ is the potential to which the particle is subjected. But for now simply think of $\psi(x,t)$ as the solution to Eq. (1).

II. Separation of Variables

Let's look for separable solutions to Eq. (1). As before we start with a product function $\psi(x,t)=X(x)T(t)$ and substitute this into Eq. (1), which yields

$$-\frac{\hbar^2}{2m}\frac{X''}{X}+V(x,t)=i\hbar\frac{T'}{T} \tag{2}$$

Now $V(x,t)$ is often independent of time, in which case Eq. (2) becomes

$$-\frac{\hbar^2}{2m}\frac{X''}{X}+V(x)=i\hbar\frac{T'}{T}. \tag{3}$$

The variables x and t are now separated; both sides of the equation are thus equal to some constant, which is conventionally called E. This gives us two ordinary differential equations that are related via the separation constant E,

$$T'(t) = -i\frac{E}{\hbar}T(t), \tag{4}$$

$$-\frac{\hbar^2}{2m}X''(x) + V(x)X(x) = EX(x). \tag{5}$$

Equation (4) says that the first derivative of T is proportional to T. The function T must thus be an exponential and is given by

$$T(t) = T_0 e^{-i\frac{E}{\hbar}t}. \tag{6}$$

As with the wave equation the time dependence is harmonic, but because Eq. (4) is a first-order equation there is only one solution, not two linearly independent solutions as in the case of the wave equation. From Eq. (6) we see that the (angular) frequency of oscillation ω equals $E/\hbar$.

III. Separable Solutions for a Free Particle

Equation (5), the differential equation for $X(x)$, has no solution until we specify the potential $V(x)$. Our interest here is in a free particle – one with no external force. Zero force implies a constant potential $V(x)$; we can thus set $V(x) = 0$.[1] Then Eq. (5) becomes

$$X''(x) + \frac{2mE}{\hbar^2}X(x) = 0, \tag{7}$$

which is our old friend, the harmonic oscillator equation! By this point you should be able to immediately write down the two independent solutions

$$X^+(x) = X_0 e^{i\sqrt{\frac{2mE}{\hbar^2}}x}, \tag{8a}$$

$$X^-(x) = X_0 e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}. \tag{8b}$$

[1] As is the case in classical mechanics, making the potential some unspecified arbitrary constant (rather than zero) does not change the physics. In the case at hand it is simplest to let that constant equal zero.

As usual, we identify the wave vector k as the factor that multiplies x in the argument of the harmonic function (excluding the $\pm i$). Thus $k = \sqrt{2mE/\hbar^2}$. Solving this equation for $E = \hbar^2 k^2/2m$ and comparing this with the expression for the frequency $\omega = E/\hbar$ gives us the dispersion relation for the free-particle SE

$$\omega(k) = \frac{\hbar k^2}{2m}. \tag{9}$$

Notice that as a function of k, this is different than

$$\omega(k) = ck, \tag{10}$$

the dispersion relation for harmonic solutions to the wave equation: the wave-equation dispersion relation is a *linear* function of k while the SE dispersion relation is a *quadratic* function of k. The significance of this difference will be discussed in a Lectures 27 and 28.

Combining the T and X pieces we obtain two linearly independent solutions to the free-particle SE

$$\psi_k^+(x,t) = \psi_0 e^{ikx} e^{-i\omega t} = \psi_0 e^{i(kx-\omega t)} = \psi_0 e^{ik[x-(\omega/k)t]}, \tag{11a}$$

$$\psi_k^-(x,t) = \psi_0 e^{-ikx} e^{-i\omega t} = \psi_0 e^{-i(kx+\omega t)} = \psi_0 e^{-ik[x+(\omega/k)t]}. \tag{11b}$$

These two solutions are harmonic waves that travel with speed $v_{ph} = \omega/k = \hbar k/2m$. (The subscript *ph* stands for phase – more on that later.) Unlike wave-equation solutions [which all move with the same speed ($v_{ph} = c$)], the propagation speed of these harmonic waves depends upon the wave vector k, with $v_{ph} \propto k$.

As defined above, the wave vector is a positive quantity. However, if we let the wave vector take on negative as well as positive values we see that $\psi_{-k}^- = \psi_k^+$. Thus we can write all the separable solutions as

$$\psi_k(x,t) = \psi_0 e^{i[kx-\omega(k)t]}. \tag{12}$$

where now $-\infty < k < \infty$, and $\omega(k)$ is still defined by Eq. (9), the dispersion relation.

IV. The Free Particle Initial Value Problem

As it turns out (and perhaps shouldn't be too surprising) we can write any solution to the free-particle SE as a linear combination of these harmonic solutions. Because the index k is continuous, the linear combination must be expressed as an integral over k,

$$\psi(x,t) = \int_{-\infty}^{\infty} dk\, C(k)\psi_k(x,t), \tag{13}$$

where $C(k)$ is the coefficient of the kth basis state $\psi_k(k,t)$. Using Eq. (12) we can rewrite Eq. (13) as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]}, \tag{14}$$

where we have set $\psi_0 = 1/\sqrt{2\pi}$.[2] As in the case of the WE, the coefficients $C(k)$ are determined by the initial conditions, but because there is only one time derivative there is only one initial condition, $\psi(x,0)$ (the value of the wave function at $t = 0$). Setting $t = 0$ in Eq. (14), we obtain

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, C(k)\, e^{ikx}. \tag{15}$$

Now this equation tells us that $C(k)$ is simply the Fourier transform of the initial condition $\psi(x,0)$. We can thus invert Eq. (15) to write

$$C(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \psi(x,0)\, e^{-ikx}. \tag{16}$$

Taken in tandem Eqs. (14) and (16) are the complete solution to the free-particle SE initial-value problem.

V. An Initial-Value-Problem Example

Let's see what happens if we start with the initial condition

$$\psi(x,0) = \psi_0 e^{-x^2/\sigma^2}, \tag{17}$$

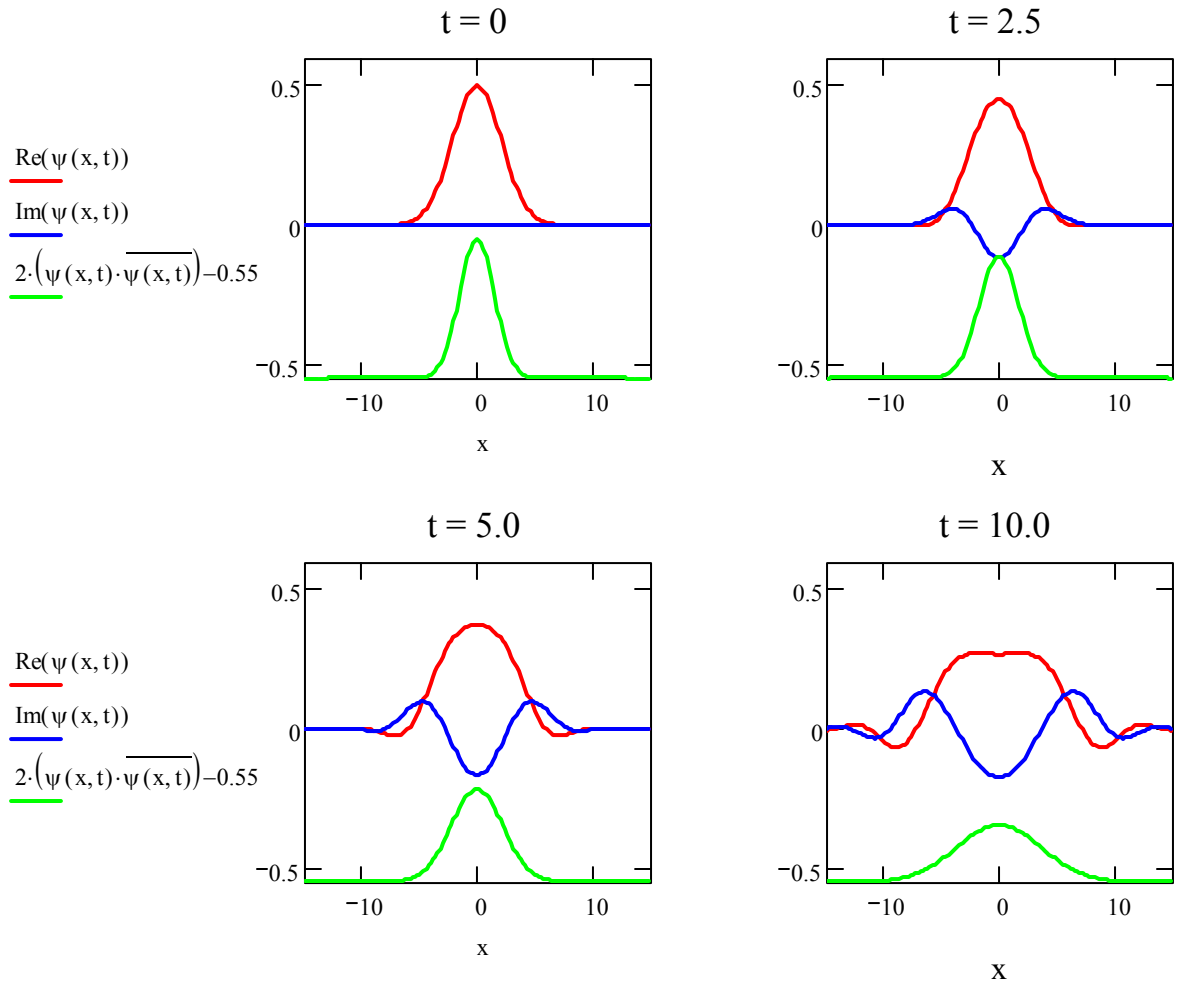
[2] The choice $\psi_0 = 1/\sqrt{2\pi}$ normalizes the harmonic basis states. See the Lecture 16 notes for details.

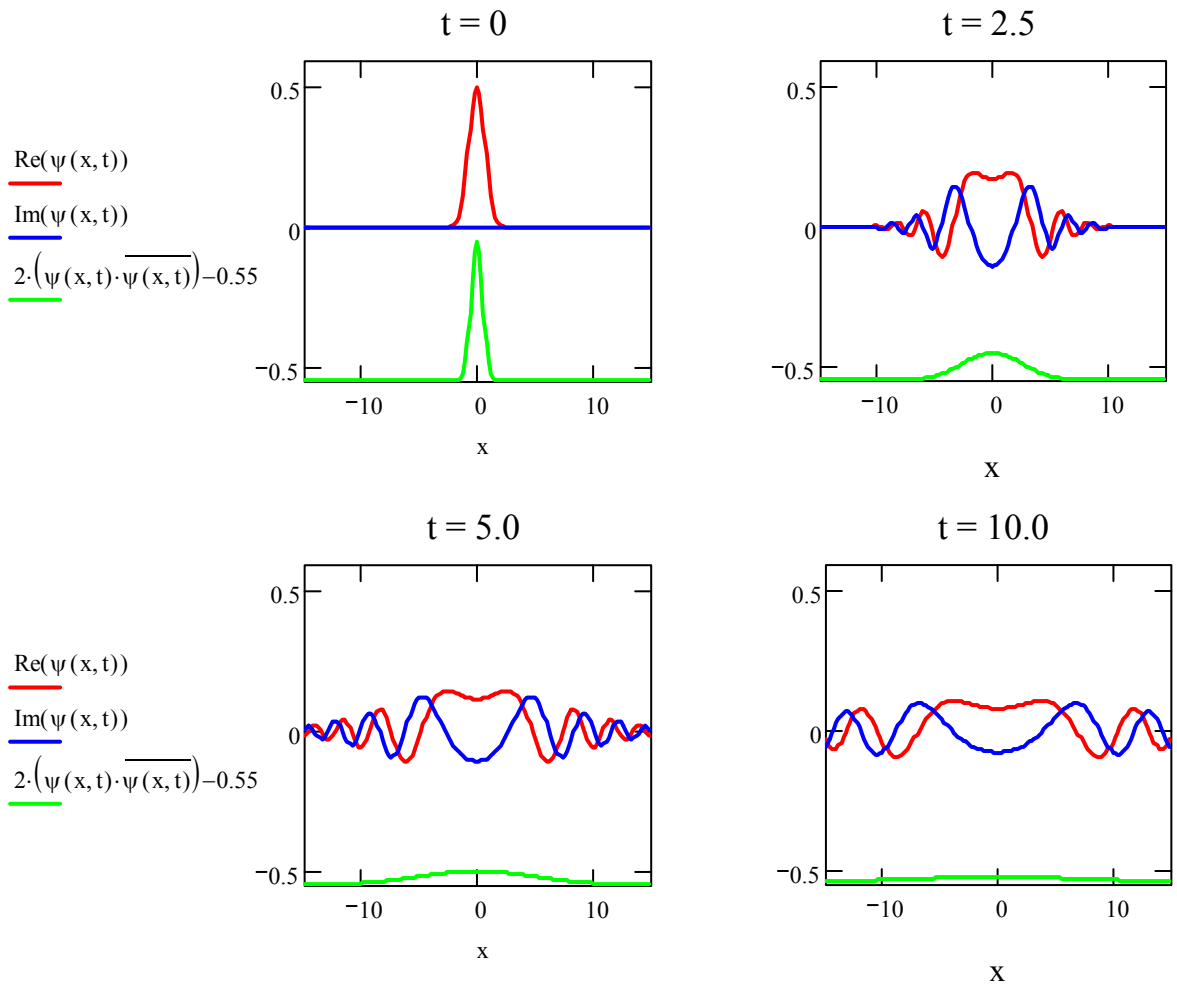
which is a Gaussian with amplitude ψ_0 and width parameter σ that is centered at the origin. As will become apparent, this corresponds to a particle whose average position $\langle x \rangle$ and average momentum $\langle p \rangle$ are both zero. Furthermore, the particle has an uncertainly in position that is proportional to the width parameter σ.

Using Eq. (16) we can calculate $C(k)$,

$$C(k) = \frac{\psi_0 \sigma}{\sqrt{2}} e^{-k^2\sigma^2/4}. \tag{18}$$

(For details of this calculation see the Lecture 12 notes.) This is pretty cool: the Fourier transform of the Gaussian function $\psi(x,0)$, $C(k)$, is also a Gaussian function (of k). Furthermore, the width parameter of $C(k)$ is $2/\sigma$, which is inversely proportional to the width parameter σ of the original function $\psi(x,0)$. Thus the product of the two width parameters is a constant, $\sigma \cdot 2/\sigma = 2$.





Using Eq. (18) in Eq. (14), we obtain the solution to this initial-value problem,

$$\psi(x,t) = \frac{\psi_0 \sigma}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dk\, e^{-k^2\sigma^2/4}\; e^{i[k\,x - \omega(k)t]}, \tag{19}$$

where $\omega(k)$ is given by Eq. (9).

The previous two figures[3] show graphs of $\mathrm{Re}\psi$, $\mathrm{Im}\psi$, and $\psi^*\psi$ (the associated probability density for the particle) for various times t. In the first figure $\sigma = 3$, while in the second figure $\sigma = 1$. As evident from the graphs of $\psi^*\psi$, in the second case the particle is initially more localized than in the first case.

The following facts are also worth noting.

[3] These figures show snapshots of the videos *SE Wavepacket 1.avi* and *SE Wavepacket 2.avi*, which are available on the class website.

(*i*) Although $\psi(x,0)$ is real, in general $\psi(x,t)$ has both real and imaginary parts. This is due to the presence of i in the Eq. (1), the SE equation.

(*ii*) Neither the real or imaginary part of $\psi(x,t)$ retains a Gaussian shape, but the probability density $\psi^*\psi$ is Gaussian for all t.

(*iii*) The wave function $\psi(x,t)$ spreads out along x in time. This is due to something known as **group-velocity dispersion** [which depends upon the dispersion relation $\omega(k)$] We will discuss this in detail later, but for now note that the *narrower* the initial pulse, the *faster* the pulse spreads in time.

Let's think for a moment about how this solution compares to the solution to the WE that has an initial Gaussian displacement (and no initial velocity). What was the solution in that case? You should recall that the initial Gaussian pulse split into two Gaussian pulses with the same width as the original displacement, and that those pulses traveled in opposite directions away from the origin at the speed c. In contrast to the solution here, the traveling pulses described by the wave equation do not broaden with time.

Exercises

***26.1** As illustrated, the solution $\psi(x,t)$ to the SE is in general a complex function. Write $\psi(x,t)$ as a sum of real and imaginary parts, $\psi_R(x,t)+i\psi_I(x,t)$, substitute into Eq. (1) and show that Eq. (1) can be written as two *real* coupled equations for ψ_R and ψ_I. (Here you will need to use the fact that the real and imaginary parts of an equation are independent of each other.)

***26.2** The momentum p of a particle in the state $\psi_k(x,t)=\psi_0 e^{i[kx-\omega(k)t]}$ is a well-defined quantity (i.e., it has no uncertainty) and is given by $p=\hbar k$. Similarly, the energy of the particle in this state is well defined and is simply the parameter $E=\hbar\omega(k)$. Using the dispersion relation $\omega(k)$, show that it is equivalent to the energy-momentum relationship for a free classical particle.

***26.3** The two linearly-independent solutions for the $X(x)$ equation were written as $X^+(x)=X_0 e^{i\sqrt{\frac{2mE}{\hbar^2}}x}$ and $X^-(x)=X_0 e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$. Find the appropriate linear combinations of these two solutions that give the other commonly used form of two linearly independent solutions: $X_1(x)=A_1\cos\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)$ and $X_2(x)=A_2\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)$.

*__26.4__ Show for the Gaussian initial condition $\psi(x,0)=\psi_0 e^{-x^2/\sigma^2}$ that the probability density $\psi^*(x,0)\psi(x,0)$ is also a Gaussian. How is the width parameter of $\psi^*(x,0)\psi(x,0)$ related to the width parameter σ of the wave function $\psi(x,0)$?

**__26.5 A Free-Particle SE Initial Value Problem__

(**a**) Starting with the initial condition

$$\psi(x,0)=\begin{cases}1/\sqrt{2} & -1<x<1\\ 0 & \text{otherwise}\end{cases}$$

for a free particle, find the function $C(k)$ appropriate to this initial condition.

(**b**) Then find the formal solution [the equivalent of Eq. (19)] to this initial value problem.

(**c**) Make plots of $\psi(x,t)$ for $t=0$, $t=2$, and $t=4$. For purposes of keeping things simple, set $\hbar=1$ and $m=1$ so that the dispersion relation is simply $\omega(k)=k^2/2$. Hint: when numerically evaluating the integral, set the limits only large enough so that the integrand is negligible at the endpoints of the integration.

(**d**) Discuss the time dependence of $\psi(x,t)$.

*__26.6__ Show that $\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]}$ with $\omega(k)=\frac{\hbar k^2}{2m}$ solves the 1D, free-particle Schrödinger equation for any $C(k)$.

***__26.7 Free Particle in 3D__. Consider the 3D, free-particle Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi=i\hbar\frac{\partial\psi}{\partial t},$$

Find separation-of-variables solutions to this equation in

(**a**) Cartesian coordinates,

(**b**) cylindrical coordinates, and

(**c**) spherical-polar coordinates.

A Propagating Wave Packet – The Group Velocity

Overview and Motivation: Last time we looked at a solution to the Schrödinger equation (SE) with an initial condition $\psi(x,0)$ that corresponds to a particle initially localized near the origin. We saw that $\psi(x,t)$ broadens as a function of time, indicating that the particle becomes more delocalized with time, but with an average position that remains at the origin. To extend that discussion of a localized wave (packet) here we look at a propagating wave packet. The two key things that we will discuss are the velocity of the wave packet (this lecture) and its spreading as a function of time (next lecture). As we shall see, both of these quantities are intimately related to the dispersion relation $\omega(k)$. This discussion has applications whenever we have localized, propagating waves, including solutions to the SE and the wave equation (WE).

Key Mathematics: Taylor series expansion of the dispersion relation $\omega(k)$ will be central in understanding how the dispersion relation is related to the properties of a propagating wave packet. The Fourier transform is again key because the localized wave packet will be described as a linear combination of harmonic waves.

I. A Propagating Schrödinger-Equation Wave Packet

In the last lecture we found the formal solution to the initial value problem for the free particle SE, which can be written as

$$\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,C(k)\,e^{i[kx-\omega(k)t]}, \tag{1}$$

where the coefficients $C(k)$ are the Fourier transform of the initial condition $\psi(x,0)$,

$$C(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\,\psi(x,0)\,e^{-ikx}, \tag{2}$$

and the dispersion relation (for the SE) is given by

$$\omega(k)=\frac{\hbar k^2}{2m}. \tag{3}$$

The example that we previously considered was for the initial condition

$$\psi(x,0)=\psi_0 e^{-x^2/\sigma^2}. \tag{4}$$

We saw that for increasing positive time $\psi(x,t)$ becomes broader (vs x), but its average position remains at the origin. So, *on average* the particle is motionless, but there is increasing probability that it will be found further away from the origin as t increases.

So you might ask, what initial condition would describe a particle initially localized at the origin, but propagating with some average velocity? Well, here is one answer:

$$\psi(x,0)=\psi_0 e^{ik_0 x}e^{-x^2/\sigma^2}. \tag{5}$$

As will be demonstrated below, you may think of k_0 as some average wave vector (or momentum $\hbar k_0$ through deBroglie's relation $p=\hbar k$) associated with the state $\psi(x,t)$.

As we did in the last lecture, let's find an expression for $\psi(x,t)$. We start by using Eq. (2) to calculate $C(k)$, so we have

$$C(k)=\frac{\psi_0}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\,e^{-x^2/\sigma^2}\;e^{-i(k-k_0)x}. \tag{6}$$

This almost looks like the Fourier transform of a Gaussian, which we can calculate.[1] Indeed, we can make it be the Fourier transform of a Gaussian if define the variable $k'=k-k_0$, so that the rhs of Eq. (6) becomes

$$\frac{\psi_0}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\,e^{-x^2/\sigma^2}\;e^{-ik'x}. \tag{7}$$

This equals the Gaussian (in the variable k')

$$\frac{\psi_0\sigma}{\sqrt{2}}e^{-k'^2\sigma^2/4}, \tag{8}$$

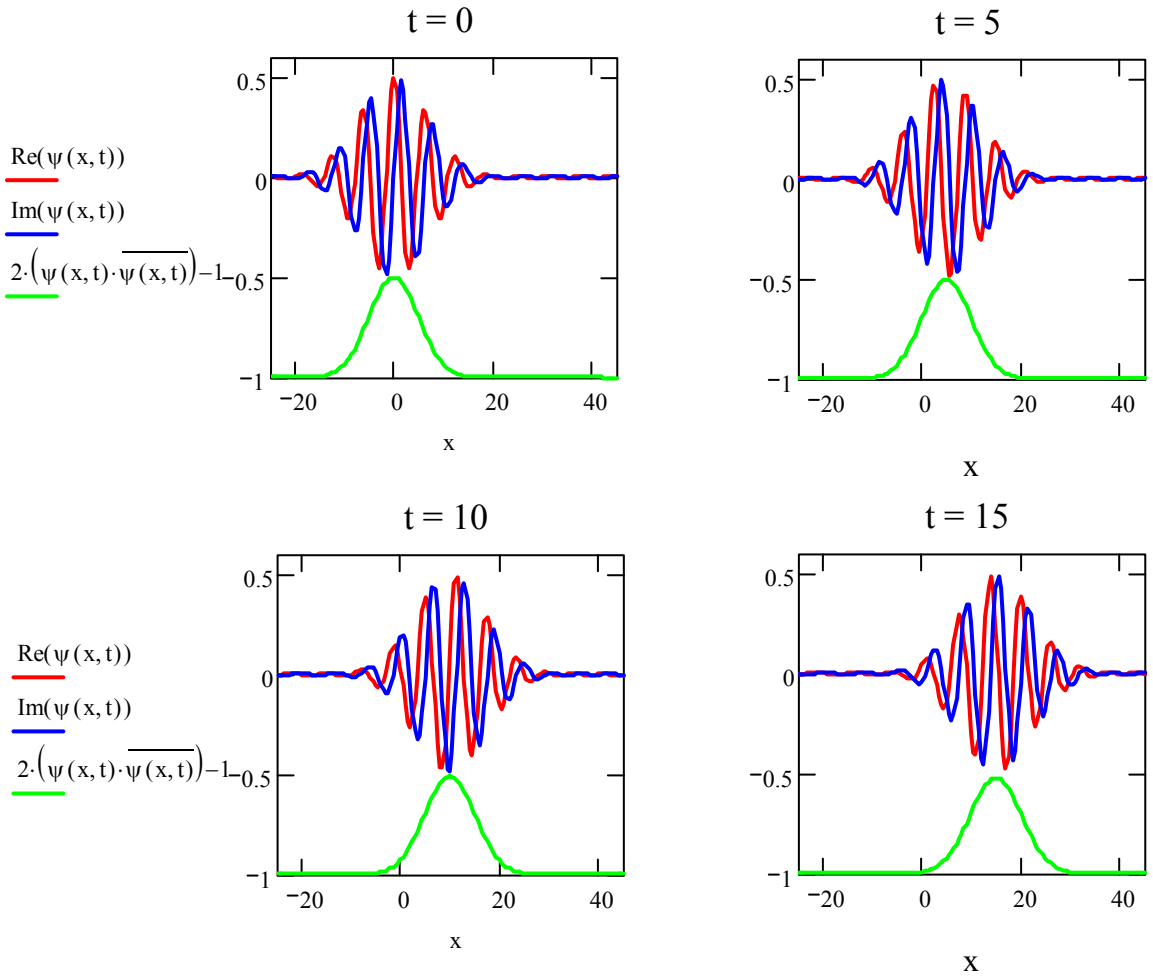
and now reusing the relation $k'=k-k_0$ we can write

$$C(k)=\frac{\psi_0\sigma}{\sqrt{2}}e^{-(k-k_0)^2\sigma^2/4}. \tag{9}$$

[1] As we stated in the last lecture, the Fourier transform of the Gaussian e^{-x^2/σ^2} is another Gaussian $\frac{\sigma}{\sqrt{2}}e^{-k^2\sigma^2/4}$.

Note that if $k_0 = 0$, then we obtain $C(k) = \left(\psi_0 \sigma/\sqrt{2}\right) e^{-k^2\sigma^2/4}$, the result from the last lecture.

Equation (9) tells us several important things. Recall that we are describing the state $\psi(x,t)$ as a linear combination of normal-mode traveling-wave states $e^{i[kx-\omega(k)t]}$, each of which is characterized by the wavevector $k = 2\pi/\lambda$ and phase velocity $v_{ph} = \omega(k)/k = \hbar k/2m$. As Eq. (1) indicates, the function $C(k)$ is the amplitude (or coefficient) associated with the state with wavevector k. As Eq. (9) indicates, the coefficients $C(k)$ are described by a Gaussian centered at the wave vector k_0. Thus, you may think of the state $\psi(x,t)$ as being characterized by an average wave vector k_0. The width of the function $C(k)$, with width parameter $2/\sigma$, is also key to describing the state $\psi(x,t)$. Because this width parameter is inversely proportional to the localization (characterized by σ) of the initial wave function $\psi(x,0)$, we see that a more localized wave function $\psi(x,0)$ requires a broader distribution (characterized by $2/\sigma$) of (normal-mode) states in order to describe it. Insofar as momentum is equal to $\hbar k$, this inverse relationship between the widths of $\psi(x,0)$ and $C(k)$ is the essence



of the uncertainty principle. We shall discuss this in great detail in Lecture 29.

Let's now look at the time dependence of $\psi(x,t)$. With Eq. (9) we can now use Eq. (1) to write

$$\psi(x,t)=\frac{\psi_0\sigma}{2\sqrt{\pi}}\int_{-\infty}^{\infty}dk\,e^{-(k-k_0)^2\sigma^2/4}\;e^{i[kx-\omega(k)t]}, \tag{10}$$

keeping in mind that the dispersion relation $\omega(k)$ is given by Eq. (3). This looks complicated, so let's look at some graphs of $\psi(x,t)$ to see what is going on with this solution. The preceding figure, which contains snapshots of the video *SE Wavepacket 3.avi*, illustrates $\psi(x,t)$ as a function of time (for a positive value of k_0). Notice that the wave packet moves in the $+x$ direction with a constant velocity. Notice also that $\psi(x,t)$ is *not* simply a translation in time of the function $\psi(x,0)$. That is, the solution is not of the form $g(x-vt)$, where v is some velocity. This can be seen in the video by noticing that the center of the wave packet travels faster than any of the individual oscillation peaks.

II. The Group Velocity

We now want to determine the velocity of the propagating wave packet described by Eq. (10). Because this solution $\psi(x,t)$ can be thought of as having an average wave vector k_0, you might guess that the velocity is simply the phase velocity $v_{ph}=\omega(k)/k$ evaluated at the average wave vector k_0. That is, you might think that the packet's velocity is simply the velocity of the normal-mode traveling-wave solution

$$\psi_{k_0}(x,t)=\psi_0 e^{i[k_0x-\omega(k_0)t]}=\psi_0 e^{ik_0[x-(\omega/k_0)t]}, \tag{11}$$

which propagates in the $+x$ direction at the phase velocity $v_{ph}=\omega(k_0)/k_0=\hbar k_0/2m$. However, this is not correct!

To figure out the packet's velocity we must carefully analyze the propagating-pulse solution described by Eq. (10). This solution lends itself to some approximation because part of the integrand, $e^{-(k-k_0)^2\sigma^2/4}$, is peaked at $k=k_0$, and for values of $|k-k_0|>>2/\sigma$ this part of the integrand is nearly zero. The importance of this is that we only need to know what $\omega(k)$ is for $|k-k_0|$ less than a few times the width parameter $2/\sigma$. That is, we only need to know what $\omega(k)$ is for values of k close to k_0. If $\omega(k)$ is does not vary too much for these values of k, then it makes sense to

approximate $\omega(k)$ by the first few terms of a Taylor series expansion about the point k_0. So we write

$$\omega(k) = \omega(k_0) + \omega'(k_0)(k-k_0) + \frac{1}{2}\omega''(k_0)(k-k_0)^2 + \ldots \tag{12}$$

If we now approximate $\omega(k)$ in Eq. (10) by the first two terms of the series, $\omega(k) \approx \omega(k_0) + \omega'(k_0)(k-k_0)$, then we obtain

$$\psi(x,t) \approx \frac{\psi_0 \sigma}{2\sqrt{\pi}} e^{-i[\omega(k_0) - \omega'(k_0)k_0]t} \int_{-\infty}^{\infty} dk\, e^{-(k-k_0)^2\sigma^2/4}\, e^{ik[x-\omega'(k_0)t]}. \tag{13}$$

This looks rather messy, but the integral can be calculated exactly to yield

$$\psi(x,t) \approx \psi_0 e^{ik_0\{x-[\omega(k_0)/k_0]t\}}\, e^{-[x-\omega'(k_0)t]^2/\sigma^2}. \tag{14}$$

We can now easily see what is going on. This (approximate) solution is the product of the normal-mode traveling wave solution $\psi_{k_0}(x,t) = \psi_0 e^{ik_0\{x-[\omega(k_0)/k_0]t\}}$ (at the wave vector k_0), which travels at a speed equal to the phase velocity

$$v_{ph}(k) = \frac{\omega(k)}{k} \tag{15}$$

(evaluated at k_0) and a Gaussian "envelope" function $e^{-[x-\omega'(k_0)t]^2/\sigma^2}$, which travels at a speed equal to $\omega'(k_0)$. The derivative $\omega'(k)$ is known as the **group velocity**

$$v_{gr}(k) = \frac{d\omega(k)}{dk} \tag{16}$$

and so the envelope function, which describes the position of the packet, travels at the group velocity (evaluated at $k = k_0$). Note that the group and phase velocities are not necessarily equal. The group velocity is typically more important than the phase velocity because the average position of the particle is given by the peak of the envelope function.

With these definitions of phase and group velocities we can now write Eq. (14) as

$$\psi(x,t) \approx \psi_0 e^{ik_0(x-v_{ph}t)}\, e^{-(x-v_{gr}t)^2/a_x^2}, \tag{17}$$

where both v_{ph} and v_{gr} are evaluated at the wave vector k_0.

III. Application to the Schrödinger Equation

You may have noticed that nothing in the last section was necessarily directly related to the SE. That is, Eq. (17) can be applied to any situation where general solutions to the problem at hand can be described as a linear combination of harmonic, traveling-wave solutions that have a dispersion relation $\omega(k)$. The SE happens to be one of those situations; so let's apply the results of the last section to the SE. We simply need to know that for the SE the dispersion relation is

$$\omega(k) = \frac{\hbar k^2}{2m}. \tag{18}$$

From Eq. (18) we obtain the phase and the group velocities $v_{ph}(k_0) = \hbar k_0/2m$ and $v_{gr}(k_0) = \hbar k_0/m$, respectively. Notice that the group velocity is twice the phase velocity. This explains the behavior of the pulse in the video, where the center of the pulse (which travels at v_{gr}) travels faster than any of the oscillation peaks (which travel at v_{ph}). With the interpretation that Eq. (10) describes a particle with an average momentum $p_0 = \hbar k_0$, we see that the group velocity corresponds to the result for a classical, nonrelativistic particle $v_{gr} = p_0/m$.

IV. Application to the Wave Equation

We can also apply the results of Sec. II to the wave equation. Because harmonic traveling waves can also be used as basis functions for solutions to the WE (see Lecture notes 21), we can also create a wave-packet solution to the WE of the form of Eq. (17). Again , we simply need to know the dispersion relation

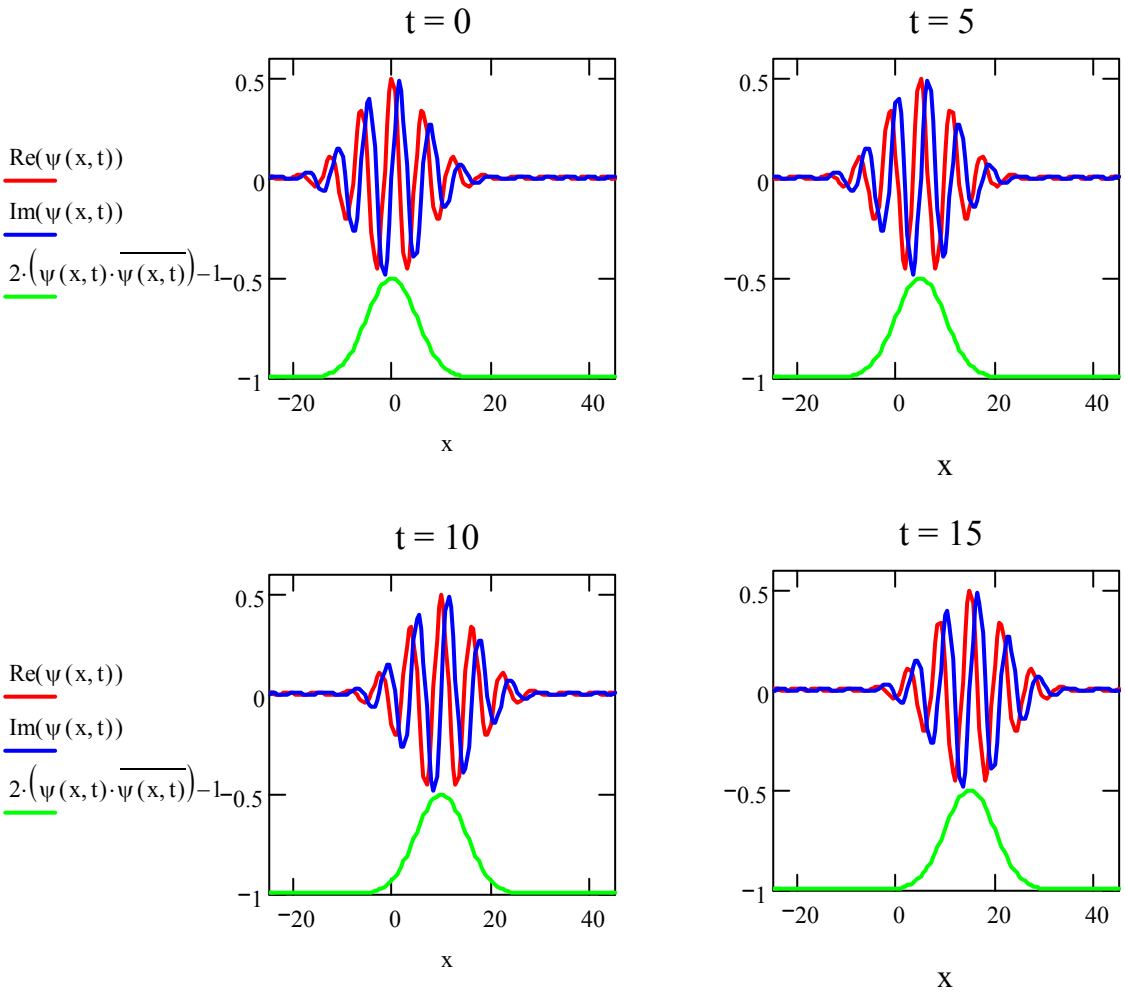
$$\omega(k) = ck \tag{19}$$

in order to calculate the phase and group velocities, which are thus $v_{ph}(k_0) = \omega(k_0)/k_0 = c$ and $v_{gr}(k_0) = \omega'(k_0) = c$, respectively. So in this case the two velocities are equal! Then the solution given by Eq. (17) becomes

$$\psi_{k_0}(x,t) = \psi_0 e^{ik_0(x-ct)} e^{-(x-ct)^2/a_x^2}. \tag{20}$$

Notice that Eq. (20) is a function of $x - ct$, and as such is an *exact* solution to the wave equation, rather than an approximate solution (as it is for the SE). (Why is that?) The

figure on the preceding page shows snapshots of the video *WE Wavepacket 1.avi*. In contrast to the SE solution both the center of the wave packet and the oscillation peaks travel at the same velocity, consistent with the solution being a function of $x - ct$.



Exercises

*__27.1__ Show that Eq. (13) follows from Eq. (10) with the linear Taylor's-series approximation described in the notes.

*__27.2__ Equation (12) is the Taylor's-series expansion of the dispersion relation about the point $k = k_0$. For the dispersion relation appropriate to the WE, find *all* terms in this expansion. Then argue why Eq. (20), is an exact solution to the WE.

****27.3 SE Approximate Solution**

(**a**) Calculate the integral on the rhs of Eq. (13) and show that Eq. (13) simplifies to Eq. (14). (Hint: Transform the integral to be the Fourier transform of a Gaussian, and then use the fact that the Fourier transform of e^{-x^2/σ^2} is $\frac{\sigma}{\sqrt{2}}e^{-k^2\sigma^2/4}$.)

(**b**) Show that Eq. (14) consistent with Eq. (5), the initial condition.

***27.4 EM Waves** For electromagnetic waves traveling in a dielectric material such as glass the dispersion relation is $\omega(k)=(c/n)k$, where n is the index of refraction, which is often assumed to be a constant.

(**a**) If n is indeed a constant, calculate the phase and group velocities for these waves.

(**b**) Often, however, the index of refraction depends upon the wave vector k. Assuming that $n(k)=n_0+n_1k$, find the phase and group velocities.

(**c**) For $n(k)$ given in (b) show that $v_{gr}=v_{ph}\left[1-n_1k/(n_0+n_1k)\right]$.

***27.5** Calculate $\psi^*\psi$ for the approximate wave function given by Eq. (17) and show that $\psi^*\psi$ travels at the group velocity v_{gr}.

A Propagating Wave Packet – Group Velocity Dispersion

Overview and Motivation: In the last lecture we looked at a localized solution $\psi(x,t)$ to the 1D free-particle Schrödinger equation (SE) that corresponds to a particle moving along the x axis (at a constant velocity). We found an approximate solution that has two velocities associated with it, the phase velocity and the group velocity. However, the approximate solution did not exhibit an important feature of the full solution – that the localization (i.e., width) of the wave packet changes with time. In this lecture we discuss this property of propagating, localized solutions to the SE.

Key Mathematics: The next term in the Taylor series expansion of the dispersion relation $\omega(k)$ will be central in understanding how the width of the pulse changes in time. We will also gain practice at looking at some complicated mathematical expressions and extracting their essential features. We will do this, in part, by defining normalized, unitless parameters that are applicable to the problem.

I. The First-Order Approximate Solution (Review)

In the last lecture we looked at a localized, propagating solution that can be described as a linear combination of traveling, normal-mode solutions of the form $e^{i[kx-\omega(k)t]}$,

$$\psi(x,t)=\frac{\psi_0\sigma}{2\sqrt{\pi}}\int_{-\infty}^{\infty}dk\,e^{-(k-k_0)^2\sigma^2/4}\,e^{i[kx-\omega(k)t]}. \tag{1}$$

If Eq. (1) is a solution to the SE, then the dispersion relation is $\omega(k)=\hbar k^2/2m$. In order to gain some insight into Eq. (1) we Taylor-series expanded the dispersion relation about the average wave vector k_0 associated with $\psi(x,t)$,

$$\omega(k)=\omega(k_0)+\omega'(k_0)(k-k_0)+\frac{1}{2}\omega''(k_0)(k-k_0)^2+\ldots. \tag{2}$$

We then approximated $\omega(k)$ by the first two terms (the constant and linear-k terms) in the expansion and obtained the approximate solution

$$\psi(x,t)\approx\psi_0 e^{ik_0\left[x-v_{ph}(k_0)t\right]}e^{-\left[x-v_{gr}(k_0)t\right]^2/\sigma^2}, \tag{3}$$

where $v_{ph}(k)=\omega(k)/k$ is known as the phase velocity and $v_{gr}(k)=\omega'(k)$ is known as the group velocity. The phase velocity is the speed of the normal-mode solution $e^{ik_0[x-(\omega(k_0)/k_0)t]}$, while the group velocity is the speed of the envelope function $e^{-[x-\omega'(k_0)t]^2/\sigma^2}$. Because it is also the speed of the probability density function

$$\psi^*\psi = \psi_0^*\psi_0\, e^{-2[x-\omega'(k_0)t]^2/\sigma^2}, \tag{4}$$

it can be though of as the average speed of the particle that the SE describes.

However, the approximate solution [Eq. (3)], does not exhibit an important property of the exact solution: the localization (or width) of the exact solution varies with time while the localization of the approximate solution is constant (and can be described by the width parameter σ.)

The three videos, *SE Wavepacket4.avi*, *SE Wavepacket5.avi*, and *SE Wavepacket6.avi* illustrate the time dependent broadening of propagation wave-packet solutions. Notice that the narrower the initial wave packet, the faster it spreads out in time. This is one result from the analysis below.

II. The Second-Order Approximate Solution

By also including the next term in Eq. (2), the Taylor's series expansion of the dispersion relation, we obtain an approximate solution that exhibits the desired feature of a width that changes as the wave packet propagates.[1] Including the first three terms in the Taylor's series expansion and substituting this into Eq. (1) produces, after a bit of algebra, the approximate solution

$$\psi(x,t) \approx \frac{\psi_0\sigma}{2\sqrt{\pi}} e^{-i[\omega(k_0)-\omega'(k_0)k_0]t} \int_{-\infty}^{\infty} dk\; e^{-(k-k_0)^2[\sigma^2/4+i\omega''(k_0)t/2]}\, e^{ik[x-\omega'(k_0)t]} \tag{5}$$

This is exactly the same as the approximate solution that we obtained in the last lecture except for the term containing $\omega''(k_0)$. But notice where it appears – as an additive term to $\sigma^2/4$, which controls the width of the pulse. Thus we might already guess that $\omega''(k_0)$ will affect the width as the pulse propagates.

Fortunately, for purposes of further analysis Eq. (5) has an analytic solution

$$\psi(x,t) \approx \frac{\psi_0\,\sigma}{\left\{\sigma^4+\left[2\omega''(k_0)t\right]^2\right\}^{1/4}} e^{-(i/2)\arctan\left[2\omega''(k_0)t/\sigma^2\right]}\, e^{2i\omega''(k_0)t[x-\omega'(k_0)t]^2/\left\{\sigma^4+[2\omega''(k_0)t]^2\right\}} \times e^{ik_0[x-(\omega(k_0)/k_0)t]}\, e^{-[x-\omega'(k_0)t]^2\Big/\left(\sigma^2\left\{1+\left[2\omega''(k_0)t/\sigma^2\right]^2\right\}\right)}. \tag{6}$$

[1] Actually, all of the higher-order terms can contribute to the broadening of the pulse. However, if the width parameter σ is not too small, then only the contribution of the quadratic term to the time dependent broadening needs to be considered.

OK, so maybe solving the integral wasn't so fortunate. But let's see what we can do with it. First notice that, compared to our previous solution we have two new exponential-function terms, $e^{-(i/2)\arctan\left(2\omega''(k_0)t/\sigma^2\right)}$ and $e^{2i\omega''(k_0)t[x-\omega'(k_0)t]^2/\left\{\sigma^4+[2\omega''(k_0)t]^2\right\}}$ [Notice that they are both equal to 1 when $\omega''(k_0)=0$.] However, because the exponents in both of these terms are purely imaginary, they contribute nothing to the width of the wave packet (as we will see below). We will thus not worry about them. The third exponential term we are already familiar with; it is the harmonic traveling wave solution $e^{ik_0[x-(\omega(k_0)/k_0)t]}$ that propagates at the phase velocity $v_{ph}(k_0)$. (Because its exponent is also purely imaginary, it too does not contribute to the width of the wave packet.)

It is the fourth exponential-function term that has some new interest for us. Notice that it is a Gaussian function that again travels with the group velocity $\omega'(k_0)$, but with a time-dependent width

$$\bar{\sigma}(t)=\sigma\left\{1+\left[\frac{2\omega''(k_0)t}{\sigma^2}\right]^2\right\}^{1/2} \tag{7}$$

that is a minimum for $t=0$. Notice that if $\omega''(k_0)=0$, as in the case of the wave equation, then the width has no time dependence and is simply σ.[2] However, in the case of the SE, for example, $\omega''(k_0)=\hbar/m\neq 0$. Thus the SE wave packet has a time dependent width.

For large times we see from Eq. (7) that $\bar{\sigma}(t)$ is approximately linear vs time

$$\bar{\sigma}(t)\approx\frac{2\omega''(k_0)t}{\sigma}, \tag{8}$$

which tells us that

$$\frac{d\bar{\sigma}(t)}{dt}\approx\frac{2\omega''(k_0)}{\sigma}. \tag{9}$$

That is, for long times the rate of broadening is proportional to the second derivative of the dispersion relation and inversely proportional to the width parameter σ. That is, the narrower the pulse is at $t=0$, the faster it broadens with time, as the videos above illustrated.

[2] Because all derivatives of the dispersion relation for the WE higher than first order are zero, Eq. (3) is exact for the wave equation.

III. Normalized Variables

To gain some further insight into this time-dependent width let's make a graph of $\bar{\sigma}(t)$ vs t. But let's be smart about the graph; let's construct the graph so that it has *universal* applicability. To do this we will graph *unitless*, *normalized* quantities that are scaled values of $\bar{\sigma}(t)$ and t. So how do we normalize $\bar{\sigma}(t)$ and t to make them universal to the problem at hand. The answer is in Eq. (7) itself. First notice that if we divide $\bar{\sigma}(t)$ by σ then we will have a unitless width that is equal to 1 at $t=0$. So let's define a normalized width σ_N as $\bar{\sigma}(t)/\sigma$. What about the variable t? Again, the answer is in Eq. (7). Notice that the quantity $2\omega''(k_0)t/\sigma^2$ is also unitless because its value squared is added to 1 in Eq. (7). So let's define a normalized time variable $\tau = 2\omega''(k_0)t/\sigma^2$. With these two universal variables Eq. (7) can be re-expressed as

$$\sigma_N(\tau) = \left[1+\tau^2\right]^{1/2} \tag{10}$$

Ah, much simpler! The figure on the next page plots $\sigma_N(\tau)$ vs τ on two different graphs with different scales. From the graphs we can visually inspect the behavior of Eq. (10). For example, we see for $\tau << 1$ that $\sigma_N(\tau) \approx 1$. This means that for $\tau << 1$ the width is approximately constant vs time. The actual time scale (in seconds) over which this is true will, of course, depend upon the parameters that went into the definition of τ: $\omega''(k_0)$ and σ. From the graph we also see that for $\tau >> 1$, $\sigma_N(\tau) \approx |\tau|$, indicating (again) that the width changes linearly vs time for large negative or positive times.

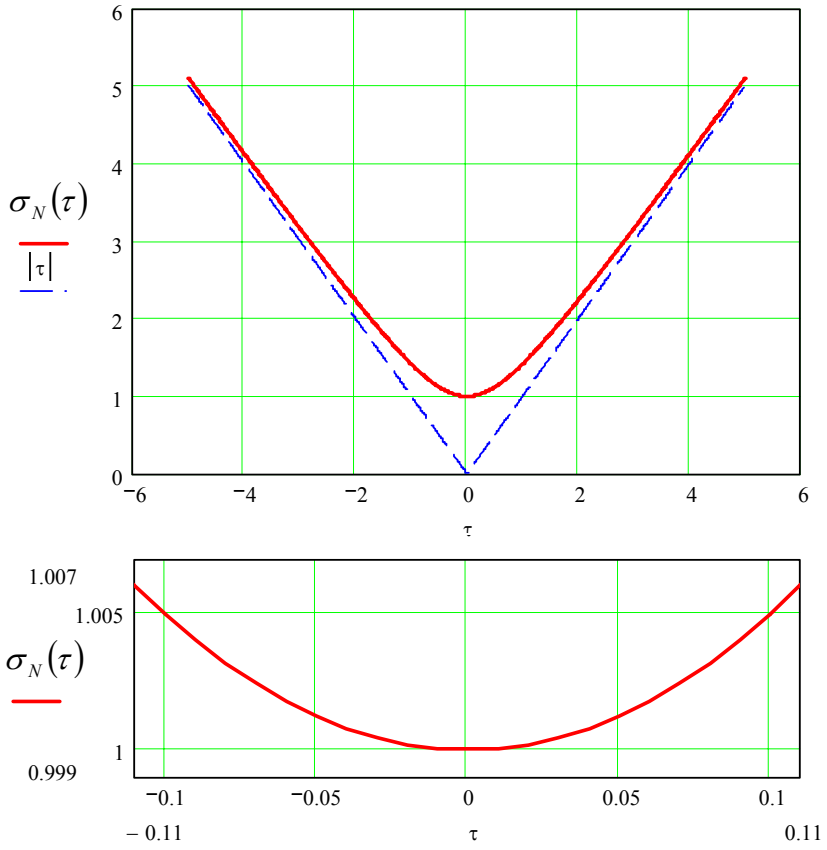
IV. Application to the Schrödinger Equation

Lastly, let's consider the probability density $\psi^*\psi$, assuming that Eq. (6) describes a solution to the SE. From Eq. (6) we calculate

$$\psi^*\psi \approx \frac{\psi_0^*\psi_0\,\sigma^2}{\left\{\sigma^4+\left[2\omega''(k_0)t\right]^2\right\}^{1/2}}\, e^{-2\left[x-\omega'(k_0)t\right]^2 \Big/ \left(\sigma^2\left\{1+\left[2\omega''(k_0)t/\sigma^2\right]^2\right\}\right)}. \tag{11}$$

Using Eq. (7), the definition of $\bar{\sigma}(t)$, Eq. (11) can be rewritten more compactly as

$$\psi^*\psi \approx \psi_0^*\psi_0 \frac{\sigma}{\bar{\sigma}(t)}\, e^{-2\left[x-\omega'(k_0)t\right]^2/\left[\bar{\sigma}(t)\right]^2}. \tag{12}$$



Notice that the probability density retains its Gaussian shape as the wave packet propagates, but with a time-dependent width parameter equal to $\bar{\sigma}(t)/\sqrt{2}$. Notice that the amplitude $\psi_0^*\psi_0\,\sigma/\bar{\sigma}(t)$ that multiplies the Gaussian function is also time dependent; as the width $\bar{\sigma}(t)$ increases this amplitude decreases. The amplitude varies with the width such that that the total probability for finding the particle anywhere along the x axis,

$$P(t)=\int_{-\infty}^{\infty} dx\,\psi^*(x,t)\psi(x,t), \tag{13}$$

remains constant in time.

The solution given by Eq. (6) and the probability density given by Eq. (11) are illustrated for both negative and positive times in the videos *SE Wavepacket7.avi*, *SE Wavepacket8.avi*, and *SE Wavepacket9.avi*. As Eq. (10) indicates, the pulse becomes narrower as $t=0$ is approached, and the pulse becomes broader after $t=0$. Notice, especially in *SE wavepacket8.avi*, that there is a time near $t=0$ during which the pulse

width is approximately constant, corresponding to $\tau << 1$. During this time the height of $\psi^*\psi$ (which is also shown in the videos) is also approximately constant.

Exercises

*__28.1__ Equation (2) is the Taylor's-series expansion of the dispersion relation about the point $k = k_0$. For the dispersion relation appropriate to the SE, find all terms in this expansion. Then argue why Eqs. (5) and (6) are exact solutions (as opposed to approximate solutions) to the SE.

**__28.2 A SE free particle__

(**a**) Rewrite Eq. (11), the expression for the probability density, with expressions for $\omega'(k)$ and $\omega''(k)$ that are appropriate for a wave described by the Schrödinger equation.

(**b**) Make several graphs (at least 3) of the probability density $\psi^*_{k_0}(x,t)\psi_{k_0}(x,t)$ vs x for several different values of t. The graphs should clearly illustrate the change in the width of the wave packet as the wave packet propagates. For simplicity you may set $\hbar = 1$ and $m = 1$.

*__28.3 The Dimensionless Time Variable τ__

(**a**) Using dimensional analysis, show that the variable $\tau = 2\omega''(k_0)t/\sigma^2$ is unitless.

(**b**) $|\tau| << 1$ and $|\tau| >> 1$ corresponds to what conditions on t?

**__28.4__ The figure in the notes shows that for $|\tau| < 0.1$ the width of the wave packet is nearly constant. Let's apply this result to a SE free electron with a kinetic energy of 10 eV. To do this find the value of t (in seconds) that corresponds to $\tau = 0.1$. Do this for values of σ = 10 nm and 10 μm. For these two cases how far does the electron travel in the time corresponding to $\tau = 0.1$? How does each of these distances compare with the respective initial width?

**__28.5 SE probability density__.

(**a**) Substitute Eq. (12) into Eq. (13), calculate the integral, and thus show that the result does not depend upon t.

(**b**) Generally, the constant ψ_0 in Eq. (12) is chosen so that the total probability to find the particle anywhere is equal to 1. Using your result in (a), find a value for ψ_0 that satisfies this condition.

*__28.6__ Show that during a normalized time interval of $\tau = 1$ the normalized distance d/σ traveled is equal to k_0/σ_k (where $\sigma_k = 2/\sigma$). As the normalized width σ_N is controlled by τ, this shows that the dispersion is controlled by the ratio k_0/σ_k.

The Uncertainty Principle

Overview and Motivation: Today we discuss our last topic concerning the Schrödinger equation, the uncertainty principle of Heisenberg. To study this topic we use the previously introduced, general wave function for a freely moving particle. As we shall see, the uncertainty principle is intimately related to properties of the Fourier transform.

Key Mathematics: The Fourier transform, the Dirac delta function, Gaussian integrals, variance and standard deviation, quantum mechanical expectation values, and the wave function for a free particle all contribute to the topic of this lecture.

I. A Gaussian Function and its Fourier Transform

As we have discussed a number of times, a function $f(x)$ and its Fourier transform $\hat{f}(k)$ are related by the two equations

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

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

We have also mentioned that if $f(x)$ is a Gaussian function

$$f(x) = e^{-x^2/\sigma_x^2}\,, \tag{2}$$

then its Fourier transform $\hat{f}(k)$ is also a Gaussian,

$$\hat{f}(k) = \frac{\sqrt{2}}{\sigma_k} e^{-k^2/\sigma_k^2}\,, \tag{3}$$

where the width parameter σ_k of this second Gaussian function is equal to $2/\sigma_x$, and so we have the result that the product $\sigma_x \sigma_k$ of the two width parameters is a constant,

$$\sigma_x \sigma_k = 2\,. \tag{4}$$

Thus, if we increase the width of one function, either $f(x)$ or $\hat{f}(k)$, the width of the other must decrease, and vice versa.

Now this result wouldn't be so interesting except that it is a general relationship between any function and it Fourier transform: as the width of one of the functions is increased, the width of the other must decrease (and vice versa). Furthermore, as we shall see below, this result is intimately related to Heisenberg's uncertainty principle of quantum mechanics.

II. The Uncertainty Principle

The uncertainty principle is often written as

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}, \tag{5}$$

where Δx is the uncertainty in the x coordinate of the particle, Δp_x is the uncertainty in the x component of momentum of the particle, and $\hbar = h/2\pi$, where h is Planck's constant. Equation (5) is a statement about *any* state $\psi(x,t)$ of a particle described by the Schrödinger equation.[1] While there are plenty of qualitative arguments concerning the uncertainty principle, today we will take a rather mathematical approach to understanding Eq. (5).

The two uncertainties Δx and Δp_x are technically the **standard deviations** associated with the quantities x and p_x, respectively. Each uncertainty is the square root of the associated **variance**, either $(\Delta x)^2$ or $(\Delta p_x)^2$, which are defined as

$$(\Delta x)^2 = \left\langle \left(x - \langle x \rangle\right)^2 \right\rangle, \tag{6a}$$

$$(\Delta p_x)^2 = \left\langle \left(p_x - \langle p_x \rangle\right)^2 \right\rangle, \tag{6b}$$

where the brackets $\langle\ \rangle$ indicate the average of whatever is inside them.

Experimentally, the quantities in Eq. (6) are determined as follows. We first measure the position x of a particle that has been prepared in a certain state $\psi(x,t)$. We must then prepare an identical particle in *exactly* the same state $\psi(x,t)$ (with time suitably shifted) and repeat the position measurement *exactly*, some number of times. We would then have a set of measured position values. From this set we then calculate the average position $\langle x \rangle$. For each measurement x we also calculate the quantity $\left(x - \langle x \rangle\right)^2$, and then find the average of this quantity. This last calculated quantity is the

[1] We are implicitly thinking about the 1D Schrödinger equation; thus there is only one spatial variable.

variance in Eq. (6a). Finally, the square root of the variance is the standard deviation Δx. This whole process is then repeated, except this time a series of momentum measurements is made, allowing one to find Δp_x.

What we want to do here, however, is use the theory of quantum mechanics to calculate the variances in Eq. (6). How do we calculate the average value of a measurable quantity in quantum mechanics? Generally, we calculate the **expectation value** of the operator associated with that quantity. For example, let's say we are interested in the (average) value of the quantity O for a particle in the state $\psi(x,t)$. We then calculate the expectation value of the associated operator $\hat{O}$, which is defined as[2]

$$\langle O \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t)\hat{O}\psi(x,t)\,dx}{\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\,dx}. \tag{7}$$

The quantity O can be any measurable quantity associated with the state: the position x, for example.

Notice that the variance involves two expectation values. Again consider the position. We see that we must first use Eq. (7) to calculate $\langle x \rangle$ and then use that in the calculation of the second expectation value. Finally to get Δx we must take the square root of Eq (6a).

We can actually rewrite Eq. (6) in slightly simpler form, as follows. Consider Eq. (6a). We can rewrite it as

$$(\Delta x)^2 = \left\langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \right\rangle \tag{8}$$

Now because the expectation value is a linear operation [see Eq. 7], this simplifies to

$$(\Delta x)^2 = \left\langle x^2 \right\rangle - \left\langle 2x\langle x \rangle \right\rangle + \left\langle \langle x \rangle^2 \right\rangle. \tag{9}$$

[2] Usually in quantum mechanics one deals with normalized wave functions, in which case the denominator of Eq. (6) is equal to 1. Rather than explicitly deal with normalized functions, we will use Eq. (7) as written.

Furthermore, because an expectation value is simply a number, $\left\langle \langle x \rangle^2 \right\rangle = \langle x \rangle^2$ and $\left\langle 2x\langle x \rangle \right\rangle = 2\langle x \rangle\langle x \rangle = 2\langle x \rangle^2$. Eq. (9) thus simplifies to

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 . \tag{10a}$$

Similarly, for $(\Delta p_x)^2$ we also have

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 . \tag{10b}$$

Thus we can write the two uncertainties as

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} , \tag{11a}$$

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} . \tag{11b}$$

III. The Uncertainty Principle for a Free Particle

A. A Free Particle State

Let's now consider a free particle and calculate these two uncertainties using Eq. (11). You should recall that we can write any free-particle state as a linear combination of normal-mode traveling wave solutions as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx - \omega(k)t]} , \tag{12}$$

where the coefficient $C(k)$ of the k th state is the Fourier transform of the initial condition $\psi(x,0)$,

$$C(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \psi(x,0)\, e^{-ikx} , \tag{13}$$

and the dispersion relation is, of course, given by $\omega(k) = \hbar k^2/2m$. To keep things simple, let's assume that the state we are interested in is a particle moving along the x axis. As discussed in the Lecture 27 notes one particular initial condition (but certainly not the only one, see Exercise 29.1) that can describe such a particle is

$$\psi(x,0) = \psi_0 e^{ik_0 x} e^{-x^2/\sigma_x^2} . \tag{14}$$

As we also saw in those notes, this initial condition results in

$$C(k) = \frac{\psi_0 \sigma_x}{\sqrt{2}} e^{-(k-k_0)^2 \sigma_x^2/4}, \tag{15}$$

which gives us the wave function

$$\psi(x,t) = \frac{\psi_0 \sigma_x}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dk\, e^{-(k-k_0)^2 \sigma_x^2/4}\; e^{i[k x - \omega(k) t]} . \tag{16}$$

B. Position Uncertainty Δx

With the wave function in Eq. (16) we can now (in principle) calculate the expectation values in Eq. (11). We start by calculating the uncertainty in x. From Eq. (11) we see that we need to calculate two expectation values: $\langle x \rangle$ and $\langle x^2 \rangle$. Using Eq. (6), the definition of an expectation value, we write the expectation value of x as

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t)\, \hat{x}\, \psi(x,t)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,t) \psi(x,t)\, dx}, \tag{18}$$

where we have kept the "hat" on the x inside the integral to emphasize that $\hat{x}$ is an operator. But when $\hat{x}$ operates on $\psi(x,t)$ it simply multiplies $\psi(x,t)$ by x. Equation (18) then becomes

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,t) \psi(x,t)\, dx} . \tag{19}$$

We could now insert Eq. (16) for $\psi(x,t)$ into Eq. (19) and calculate away, but it will get really ugly really fast. But let's recall the behavior of the free particle state described by Eq. (16): As it propagates from negative time it gets narrower up until $t = 0$, and then as it further propagates it becomes broader. Given this, let's calculate the uncertainty in x when it will be a minimum, at $t = 0$.

Then Eq. (19) becomes[3]

$$\langle x\rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,0)\, x\, \psi(x,0)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,0)\psi(x,0)\, dx}. \tag{20}$$

If we now insert the rhs of Eq. (14), the expression for $\psi(x,0)$, into Eq. (20) we get

$$\langle x\rangle = \frac{\int_{-\infty}^{\infty} x\, e^{-2x^2/\sigma_x^2}\, dx}{\int_{-\infty}^{\infty} e^{-2x^2/\sigma_x^2}\, dx} \tag{21}$$

You should immediately recognize that the integral in the numerator is zero (why?) and that the integral in the denominator is not zero. Thus, $\langle x\rangle = 0$ and so $\langle x\rangle^2 = 0$. This result should not be very surprising: at $t = 0$ the probability density is a Gaussian centered at $x = 0$, so the average value of the position is simply zero.

We now calculate $\langle x^2\rangle$, which is given by

$$\langle x^2\rangle = \frac{\int_{-\infty}^{\infty} \psi^*(x,0)\, x^2\, \psi(x,0)\, dx}{\int_{-\infty}^{\infty} \psi^*(x,0)\psi(x,0)\, dx}. \tag{22}$$

As we did in calculating $\langle x\rangle$ we substitute the rhs of Eq. (14) for $\psi(x,0)$, which gives us

[3] As far as all the calculations of the expectation values (that we are interested in) are concerned, t is just a parameter. We are free to simply set it to whatever value we might be interested in and calculate all expectation values with it set to that value. This would not be true if we were interested in a t dependent operator (such as the energy operator $i\hbar\,\partial/\partial t$).

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 \, e^{-2x^2/\sigma_x^2} \, dx}{\int_{-\infty}^{\infty} e^{-2x^2/\sigma_x^2} \, dx}. \tag{23}$$

Now this expectation value is certainly not zero. By looking these two integrals up in an integral table (or using Mathcad, for example) we obtain the result

$$\langle x^2 \rangle = \frac{\sigma_x^2}{4} \tag{24}$$

Given that $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ and $\langle x \rangle = 0$, we thus have

$$\Delta x = \frac{\sigma_x}{2}. \tag{25}$$

That is, the uncertainty in position is simply equal to half of the width parameter σ_x. Again, this should not be too surprising: the more spread out the wave function $\psi(x,t)$ (which is controlled by σ_x at $t = 0$) the larger the uncertainty in its position.

C. Momentum Uncertainty Δp_x

We now calculate the momentum uncertainty Δp_x. Referring to Eq. (11), we see that we need to calculate $\langle p_x \rangle$ and $\langle p_x^2 \rangle$. Notice that both of these are the expectation values of some power of the momentum. Now you should have learned in your modern physics course that the momentum operator is given by the differential operator

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}. \tag{26}$$

This then implies for any integer n that

$$\hat{p}_x^n = \left(-i\hbar \frac{\partial}{\partial x} \right)^n = (-i\hbar)^n \frac{\partial^n}{\partial x^n}.$$

Before we go ahead and do the calculations of $\langle p_x \rangle$ and $\langle p_x^2 \rangle$, it is worth considering the expectation value $\langle p_x^n \rangle$ for any integer n,

$$\left\langle p_x^n \right\rangle = \frac{(-i\hbar)^n \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\partial^n \psi(x,t)}{\partial x^n} dx}{\int_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\, dx}. \tag{27}$$

To do this we use Eq. (12), which is the general form of $\psi(x,t)$ for a free particle. (Thus this calculation will be applicable to any time t.) Substituting this into Eq. (27) gives us

$$\left\langle p_x^n \right\rangle = \frac{\frac{(-i\hbar)^n}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk'\, C^*(k')\, e^{-i[k'x-\omega(k')t]} \frac{\partial^n}{\partial x^n} \left(\int_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]} \right)}{\frac{1}{2\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk'\, C^*(k')\, e^{-i[k'x-\omega(k')t]} \int_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]}} \tag{28}$$

Now we have seen these sorts of integrals before. You may remember that things can sometimes get considerably simpler if we do some switching of the order of integration. Calculating the derivatives in the numerator and then moving the x integral to the interior (in both the numerator and denominator) produces

$$\left\langle p_x^n \right\rangle = \frac{\frac{\hbar^n}{2\pi} \int_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t} \int_{-\infty}^{\infty} dk\, k^n C(k) e^{-i\omega(k)t} \int_{-\infty}^{\infty} dx\, e^{i(k-k')x}}{\frac{1}{2\pi} \int_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t} \int_{-\infty}^{\infty} dk\, C(k) e^{-i\omega(k)t} \int_{-\infty}^{\infty} dx\, e^{i(k-k')x}} \tag{29}$$

We now use an expression for the Dirac delta function,

$$\delta(k-k') = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\, e^{i(k-k')x}, \tag{30}$$

to rewrite Eq. (29) as

$$\left\langle p_x^n \right\rangle = \frac{\hbar^n \int_{-\infty}^{\infty} dk\, k^n\, C(k) e^{-i\omega(k)t} \int_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t}\, \delta(k-k')}{\int_{-\infty}^{\infty} dk\, C(k) e^{-i\omega(k)t} \int_{-\infty}^{\infty} dk'\, C^*(k') e^{i\omega(k')t}\, \delta(k-k')}, \tag{31}$$

where we have also switched the order of the k and k' integrations. The k' integral is now trivially done, giving

$$\left\langle p_x^n \right\rangle = \frac{\hbar^n \int_{-\infty}^{\infty} dk\, C^*(k) k^n\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{32}$$

Notice that even though we started with the general, time-dependent, free-particle wave function $\psi(x,t)$ in Eq. (27), the expectation value of any (integer) power of the momentum is *independent* of time. Perhaps this should not be too surprising. For a classical free particle there is no change in momentum of the particle. Here we see for a quantum-mechanical particle that the expectation value associated with any (integer) power of the momentum does not change with time. In fact, the expectation value of *any* function of the momentum is independent of time for the free particle.

Let's now calculate Δp_x using Eq. (32). We first calculate $\langle p_x \rangle$, which is given by

$$\left\langle p_x \right\rangle = \frac{\hbar \int_{-\infty}^{\infty} dk\, C^*(k) k\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{33}$$

And using Eq. (15), the particular expression for $C(k)$ in the case at hand, Eq. (33) becomes

$$\langle p_x \rangle = \frac{\hbar \int_{-\infty}^{\infty} dk\, k\, e^{-2(k-k_0)^2 \sigma_x^2/4}}{\int_{-\infty}^{\infty} dk\, e^{-2(k-k_0)^2 \sigma_x^2/4}}. \tag{34}$$

The integrals can be simplified with the change of variable $k' = k - k_0$, $dk' = dk$, which produces

$$\langle p_x \rangle = \frac{\hbar \int_{-\infty}^{\infty} dk' (k' + k_0) e^{-2k'^2 \sigma_x^2/4}}{\int_{-\infty}^{\infty} dk'\, e^{-2k'^2 \sigma_x^2/4}}. \tag{35}$$

Bu inspection it should be clear that this simplifies to

$$\langle p_x \rangle = \hbar k_0 . \tag{36}$$

So we see that the average momentum of the particle is just the momentum of the state at the center of the distribution $C(k)$.

We lastly need to calculate $\langle p_x^2 \rangle$. However, it is actually much simpler if we directly calculate $(\Delta p_x)^2 = \langle (p_x - \langle p_x \rangle)^2 \rangle = \langle (p_x - \hbar k_0)^2 \rangle$, which we can write as

$$(\Delta p_x)^2 = \frac{\hbar^2 \int_{-\infty}^{\infty} dk\, C^*(k)(k-k_0)^2 C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{37}$$

And again using Eq. (15), the expression for $C(k)$, Eq. (37) becomes

$$(\Delta p_x)^2 = \frac{\hbar^2 \int_{-\infty}^{\infty} dk (k-k_0)^2 e^{-2(k-k_0)^2 \sigma_x^2/4}}{\int_{-\infty}^{\infty} dk\, e^{-2(k-k_0)^2 \sigma_x^2/4}}. \tag{38}$$

Making the same change of integration variable as before, $k' = k - k_0$, $dk' = dk$ (in both integrals), Eq. (38) becomes

$$(\Delta p_x)^2 = \frac{\hbar^2 \int_{-\infty}^{\infty} dk\, k'^2\, e^{-2k'^2\sigma_x^2/4}}{\int_{-\infty}^{\infty} dk\, e^{-2k'^2\sigma_x^2/4}}. \tag{39}$$

Notice that these integral are essentially the same as in Eq. (23), where we calculated $\langle x^2 \rangle$. Looking them up in the same table as before, we find that

$$(\Delta p_x)^2 = \frac{\hbar^2}{\sigma_x^2}. \tag{41}$$

and so

$$\Delta p_x = \frac{\hbar}{\sigma_x}. \tag{42}$$

Combining this with Eq. (25) for Δx we have, for our particular state at $t = 0$,

$$\Delta x\, \Delta p_x = \frac{\hbar}{2} \tag{43}$$

Notice that this is actually the *minimum* value allowed by the uncertainty principle. If you think about our traveling wave packet, you will realize that this minimum occurs only at $t = 0$: as discussed above the uncertainty in momentum is time independent but we know that the packet is narrowest in x space at $t = 0$. Thus, the minimum uncertainty product only occurs at $t = 0$. Furthermore, *the minimum uncertainty is only seen when $C(k)$ is a Gaussian distribution.* For other forms of $C(k)$, the minimum uncertainty condition is not possible.

Lastly, we make an observation concerning the coefficients $C(k)$. Consider, for example, the expectation value

$$\langle p_x \rangle = \frac{\hbar \int_{-\infty}^{\infty} dk\, C^*(k) k\, C(k)}{\int_{-\infty}^{\infty} dk\, C^*(k) C(k)}. \tag{44}$$

Notice the striking similarity of this equation and Eq. (19) for $\langle x \rangle$. Because of this similarity and because we interpret $\psi^*\psi$ as the probability density in x (real) space, we can interpret C^*C as the probability density in k space. Further, because $\hbar k$ is the momentum of the state $e^{i[kx-\omega(k)t]}$, the product C^*C is essentially the *probability density in momentum space*.

We also emphasize that while $\psi^*(x,t)\psi(x,t)$ depends upon time, the product $C^*(k)C(k)$ is time independent (for the free particle). That is, the momentum probability density is time independent. This is the basic reason that functions of the momentum operator have time-independent expectation values, as discussed above.

D. The Fourier Transform and the Uncertainty Principle

So what does the Fourier transform have to do with the uncertainty principle? Well, first recall that the functions $\psi(x,0)$ and $C(k)$ are a Fourier transform pair and that the product of their widths parameters is $\sigma_x \sigma_k = 2$. Now $\Delta x = \sigma_x/2$, and because $\Delta p_x = \hbar/\sigma_x$ we can also write $\Delta p_x = \hbar\, \sigma_k/2$. Thus we have (at $t = 0$)

$$\Delta x \Delta p_x = \hbar \frac{\sigma_x}{2} \frac{\sigma_k}{2} \tag{45}$$

That is, the products of the uncertainties associated with the $t = 0$ state is intimately related to the products of the width parameters that govern the Fourier transform pair $\psi(x,0)$ and $C(k)$.

Exercise

29.1 **Uncertainty Principle for a Different Wave Packet. Consider an alternate wave-packet initial condition for the 1D free-particle Schrödinger equation,

$$\psi(x,0) = e^{ik_0 x} e^{-\alpha|x|}.$$

(**a**) Find the function $C(k)$ that corresponds to this initial condition.
(**b**) Plot $C(k)$ for k in the vicinity of k_0, and thus argue that the average value of k is indeed equal to k_0. Note that this is equivalent to the average momentum $\langle p_x \rangle$ being equal to $\hbar k_0$.
(**c**) As was done in the notes, find the expectation values $\langle x \rangle$ and $\langle x^2 \rangle$ at $t = 0$. Thus calculate Δx, the uncertainty in x, at $t = 0$.
(**d**) Using the result from (b) for $\langle p_x \rangle$, calculate $(\Delta p_x)^2 = \left\langle \left(p_x - \langle p_x \rangle\right)^2 \right\rangle$, and from this find the uncertainty Δp_x.
(**e**) Find the $t = 0$ product $\Delta x \Delta p_x$. Does the product satisfy the uncertainty principle? What do you expect to happen to the product $\Delta x \Delta p_x$ for values of $t \neq 0$?

Divergence and Curl

Overview and Motivation: In the upcoming two lectures we will be discussing Maxwell's equations. These equations involve both the divergence and curl of two vector fields, the electric field $\mathbf{E}(\mathbf{r},t)$ and the magnetic field $\mathbf{B}(\mathbf{r},t)$. Here we discuss some details of the divergence and curl.

Key Mathematics: The aim here is to gain some insight into the physical meanings of the divergence and curl of a vector field. We will also state some useful identities concerning these two quantities.

I. Review of "del"

We have already discussed the differential object ∇ (sometimes called "del"). In Cartesian coordinates ∇ can be written as

$$\nabla = \frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial z}\hat{\mathbf{z}}. \tag{1}$$

We have seen that this object can operate on a scalar function (or scalar field) $f(\mathbf{r})$ to produce the **gradient** of $f(\mathbf{r})$, denoted $\nabla f(\mathbf{r})$. If f is expressed as a function of Cartesian coordinates, then the gradient can be written as

$$\nabla f(x,y,x) = \frac{\partial f}{\partial x}\hat{\mathbf{x}} + \frac{\partial f}{\partial y}\hat{\mathbf{y}} + \frac{\partial f}{\partial z}\hat{\mathbf{z}} \tag{2}$$

Recall that $\nabla f(\mathbf{r})$ points in the direction of the greatest change in $f(\mathbf{r})$ and is perpendicular to surfaces of constant $f(\mathbf{r})$. Recall also that $\nabla f(\mathbf{r})$ is a vector function (or vector field), which assigns a vector to each point $\mathbf{r}$ in real space.

We have also previously used ∇ on a vector function $\mathbf{V}(\mathbf{r})$ to calculate the **divergence** of $\mathbf{V}(\mathbf{r})$, denoted $\nabla \cdot \mathbf{V}(\mathbf{r})$. If $\mathbf{V}$ is expressed as a function of Cartesian coordinates, then the divergence can be written as

$$\nabla \cdot \mathbf{V}(x,y,z) = \frac{\partial V_x(x,y,z)}{\partial x} + \frac{\partial V_y(x,y,z)}{\partial y} + \frac{\partial V_z(x,y,z)}{\partial z} \tag{3}$$

Recall that $\nabla \cdot \mathbf{V}(\mathbf{r})$ is a scalar function.

A special case is the divergence of a vector field that is itself the gradient of a scalar function, $\nabla \cdot [\nabla f(\mathbf{r})]$. In this case the vector field is ∇f and so Eq. (3) becomes

$$\nabla \cdot [\nabla f(x,y,z)] = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}, \tag{4}$$

which in coordinate-system-independent notation we also write as $\nabla^2 f$.

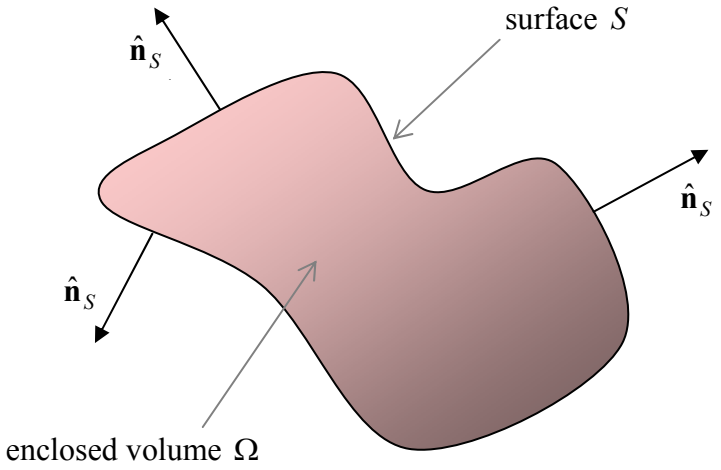
It may not be obvious, but one reason that the gradient and divergence are useful is that they are coordinate-system independent quantities. That is, as functions of position vector **r** they produce a quantity that exists independent of the coordinate system used to calculate them. However, this does *not* mean, for example, that the divergence of a vector field will be have the same functional form in each coordinate system. For example, consider the function that is equal to the distance from some reference point, the origin say. This function will have the form $\sqrt{x^2+y^2+z^2}$ when expressed in Cartesian coordinates, $\sqrt{\rho^2+z^2}$ when expressed in cylindrical coordinates, and simply r when expressed in spherical coordinates.

II. Interpretation of the Divergence.

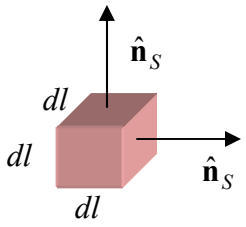
Although we previously defined the divergence of a vector function, we did not spend much (if any) time on its meaning. Let's see what we can say about $\nabla \cdot \mathbf{V}(\mathbf{r})$. To gain some insight into the divergence, let's consider the **divergence theorem**

$$\int_{\Omega} \nabla \cdot \mathbf{V}(\mathbf{r}) dv = \oint_{S} \mathbf{V}(\mathbf{r}_S) \cdot \hat{\mathbf{n}}_S(\mathbf{r}_S) dS, \tag{5}$$

which applies to a vector field $\mathbf{V}(\mathbf{r})$ defined both inside and on a closed surface S, as illustrated



In words, this equation says that the volume integral (over some volume Ω) of the divergence of a vector field $\mathbf{V}(\mathbf{r})$ equals the integral over the surface S enclosing that volume of the normal component of that same vector field $\mathbf{V}(\mathbf{r})$. Note that $\hat{\mathbf{n}}_S(\mathbf{r}_S)$ is a unit-vector field that is only defined on the surface S, and at every point on S it points *outward* and is normal to the surface. Now this theorem is true for any volume, but let's think about Eq. (5) when the volume is infinitesimally small. In fact, let's think about a cubic infinitesimal volume $dv = dl^3$, as shown.



If the volume is small enough (and the vector field is not too pathological) then we can consider $\nabla\cdot\mathbf{V}(\mathbf{r})$ to be approximately constant within the volume dl^3. On each face of the cube (with area dl^2) we can also consider $\mathbf{V}(\mathbf{r}_S)\cdot\hat{\mathbf{n}}_S = V_\perp(\mathbf{r}_S)$ to be constant. Then Eq. (5) can be rewritten approximately as

$$\nabla\cdot\mathbf{V}(\mathbf{r})dl^3 = \sum_{\substack{6\ faces\\(n)}} V_{\perp,n}(\mathbf{r}_S)dl^2 \tag{6}$$

or

$$\nabla\cdot\mathbf{V}(\mathbf{r}) = \frac{1}{dl^3}\sum_{\substack{6\ faces\\(n)}} V_{\perp,n}(\mathbf{r}_S)dl^2\ . \tag{7}$$

The quantity $V_{\perp,n}(\mathbf{r}_S)dl^2$ is usually interpreted as the **flux** of $\mathbf{V}$ (or total amount of $\mathbf{V}$) passing through the surface n with area dl^2. So what does Eq. (7) tell us? It tells us that the divergence of $\mathbf{V}(\mathbf{r})$ is equal to the *net* flux of $\mathbf{V}$ leaving the volume / unit volume. Thus, if the divergence of $\mathbf{V}$ is zero, then there is as much $\mathbf{V}$ pointing into the infinitesimal volume as is pointing out of the volume, or the net flux of $\mathbf{V}$ through the surface is zero. If the divergence of $\mathbf{V}$ is positive, then we say that there is a **source** of $\mathbf{V}$ within the volume. Conversely, if the divergence of $\mathbf{V}$ is negative, we say that there is a **sink** of $\mathbf{V}$ within the volume.

As we shall discuss in more detail shortly, one of Maxwell's equations is

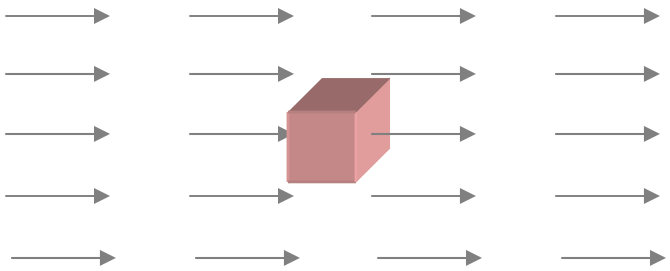
$$\nabla \cdot \mathbf{E}(\mathbf{r}) = \frac{\rho(\mathbf{r})}{\varepsilon_0}, \tag{8}$$

where $\mathbf{E}(\mathbf{r})$ is the electric field and $\rho(\mathbf{r})$ is the charge density. With our discussion above we see that the charge density is either a source (if positive) or sink (if negative) of electric field. If we are in a region of space without any charge density, then $\nabla \cdot \mathbf{E}(\mathbf{r}) = 0$, which tells us that for any volume there is as much $\mathbf{E}$ pointing inwards as outwards.

Example 1 To get a feeling for the divergence we apply Eq. (7) to a vector field to find its divergence. Let's consider a simple vector field,

$$\mathbf{V}(x, y, z) = V_0 \hat{\mathbf{x}}, \tag{9}$$

a constant vector field that points in the x direction. At each point in space this vector field is exactly the same, as the following drawing shows (positive x is to the right).

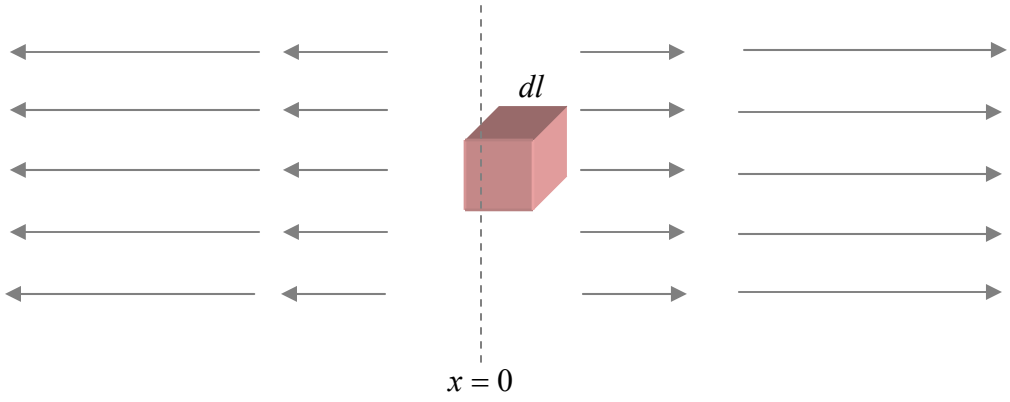


We now consider the flux coming out of each side of our infinitesimal volume dl^3. For the four sides that are parallel to the field there is no flux. One of the remaining sides has a flux equal to $V_0\, dl^2$ and other has $-V_0\, dl^2$, making the net flux emerging from the surface equal to zero. Via Eq. (7) we thus see that the divergence of this field is zero. We could, of course, have used Eq. (3) to directly calculate $\nabla \cdot \mathbf{V}(x, y, z)$, obtaining $\nabla \cdot \mathbf{V}(x, y, z) = 0$, in agreement with our analysis using Eq. (7).

Example 2 Let's look at a slightly more complicated field,

$$\mathbf{V}(x, y, z) = V_0 x \hat{\mathbf{x}}. \tag{10}$$

A graphical representation of this field would look something like the following picture.



Again, let's use Eq. (7) to calculate $\nabla\cdot\mathbf{V}(x,y,z)$. As we shall see below, the divergence is the same everywhere for this field, so for simplicity we consider a cube oriented as shown with one side at $x=0$. In this case only the right-hand-side (at $x=dl$) has any net flux, which is equal to $V_0\,dl^3$, and so via Eq. (7) we have that the divergence is simply V_0. As in Example 1, we could have directly used Eq. (3), also producing $\nabla\cdot\mathbf{V}(x,y,z)=V_0$, which is indeed independent of position.

III. The Curl and its Interpretation

Another useful first-derivative function of a vector field $\mathbf{V}(\mathbf{r})$ is known as the **curl** of $\mathbf{V}(\mathbf{r})$, usually denoted $\nabla\times\mathbf{V}(\mathbf{r})$. It has this notation due to its similarity to the cross product of two vectors. Indeed, in Cartesian coordinates it is expressed as

$$\nabla\times\mathbf{V}(x,y,z)=\left(\frac{\partial V_z}{\partial y}-\frac{\partial V_y}{\partial z}\right)\hat{\mathbf{x}}+\left(\frac{\partial V_x}{\partial z}-\frac{\partial V_z}{\partial x}\right)\hat{\mathbf{y}}+\left(\frac{\partial V_y}{\partial x}-\frac{\partial V_x}{\partial y}\right)\hat{\mathbf{z}} \tag{11}$$

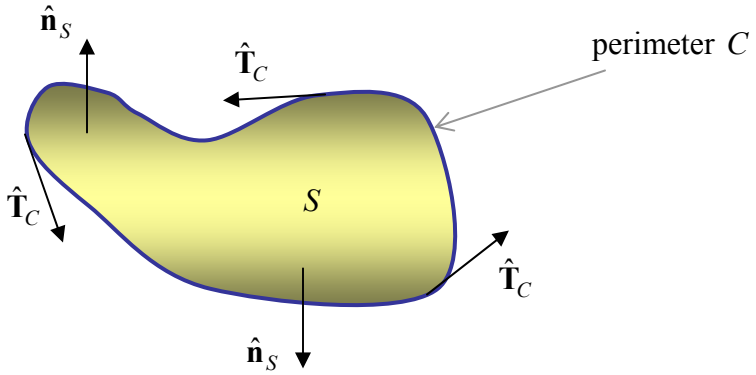
Notice that $\nabla\times\mathbf{V}(\mathbf{r})$ is itself a vector function of $\mathbf{r}$. As with the gradient and divergence, the curl is an object that is independent of the coordinate system that is used to calculate it. An easy way to remember $\nabla\times\mathbf{V}(\mathbf{r})$ in Cartesian coordinates is to see that Eq. (10) can be written as a "determinant"

$$\nabla\times\mathbf{V}(x,y,z)=\begin{vmatrix}\hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}}\\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z}\\ V_x & V_y & V_z\end{vmatrix}. \tag{12}$$

So what is the interpretation of $\nabla\times\mathbf{V}(\mathbf{r})$? Again, we appeal to a theorem of multivariable calculus, **Stoke's theorem** in this case, which can be written as

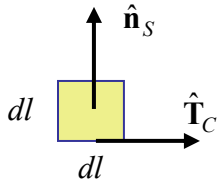
$$\int_S [\nabla\times\mathbf{V}(\mathbf{r}_S)]\cdot\hat{\mathbf{n}}_S(\mathbf{r}_S)\,dS = \oint_C \mathbf{V}(\mathbf{r}_C)\cdot\hat{\mathbf{T}}_C(\mathbf{r}_C)\,dC \tag{13}$$

In words this says that surface integral of the normal component of the curl of a vector field $\mathbf{V}(\mathbf{r}_S)$ equals the line integral around the perimeter (of that surface) of the tangential component of that same vector field $\mathbf{V}(\mathbf{r})$.



As illustrated above, $\hat{\mathbf{n}}_S(\mathbf{r}_S)$ is again a field of unit vectors that is only defined on the surface S, but this time the surface is an *open* surface so there is no outward direction. Because of this lack of outwardness, one must arbitrarily pick one side of the surface for the field $\hat{\mathbf{n}}_S(\mathbf{r})$ to point from. Similarly, $\hat{\mathbf{T}}_C(\mathbf{r}_C)$ is a unit-vector field that is only defined on the perimeter curve C. It is **tangent** to the curve C at all points along C. Its direction is found by the "right-hand rule" whereby one's thumb points along the unit vector field $\hat{\mathbf{n}}_S(\mathbf{r}_S)$ and one's fingers curl (hum…) in the direction of the field $\hat{\mathbf{T}}_C(\mathbf{r}_C)$.

To use Stoke's theorem to gain some insight into the curl, lets consider the surface to be an infinitesimal, flat, square surface with sides of length dl, as shown. One normal vector $\hat{\mathbf{n}}_S(\mathbf{r}_S)$ and one tangential vector $\hat{\mathbf{T}}_C(\mathbf{r}_C)$ associated with this surface are also shown.



Because of the infinitesimal nature of the surface we can take $\nabla\times\mathbf{V}(\mathbf{r}_S)$ to be constant on this surface, and so we can rewrite Eq. (13) as

$$\left[\nabla\times\mathbf{V}(\mathbf{r}_S)\right]_\perp dl^2 = \sum_{\substack{4\,sides\\(n)}} V_{\parallel,n}(\mathbf{r}_C)dl \tag{14}$$

or

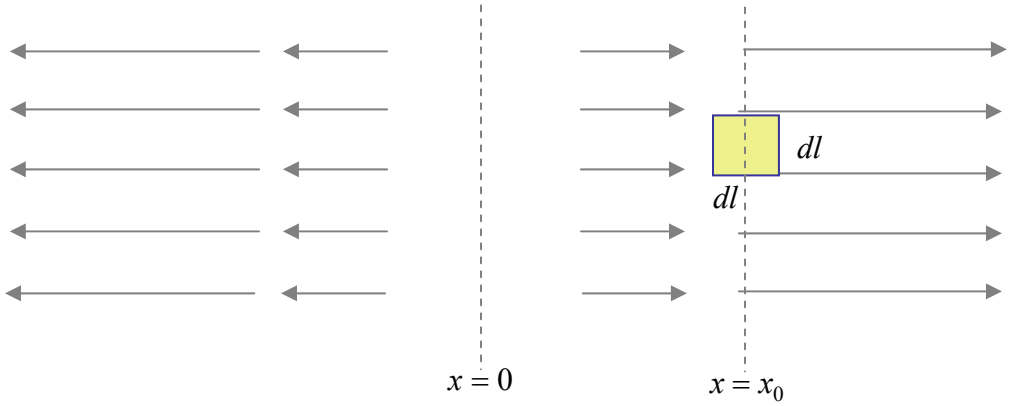
$$\left[\nabla\times\mathbf{V}(\mathbf{r})\right]_\perp = \frac{1}{dl^2}\sum_{\substack{4\,sides\\(n)}} V_{\parallel,n}(\mathbf{r})dl\,. \tag{15}$$

The quantity on the rhs of Eq. (15) is know as the **circulation** of $\mathbf{V}(\mathbf{r})$ around the curve C. So what does Eq. (15) tell us? This equation tells us that component of $\nabla\times\mathbf{V}(\mathbf{r})$ normal to an infinitesimal area is equal to the circulation of $\mathbf{V}(\mathbf{r})$ around the perimeter of that area.

Example 1 Well, maybe that last statement is just words to you. So let's do some examples to see if we can get a feel for the curl. Let's first consider the vector field that we discussed above in connection with the divergence,

$$\mathbf{V}(x,y,z) = V_0 x\,\hat{\mathbf{x}}\,. \tag{16}$$

We now consider an infinitesimal, square loop lying in the $x-y$ plane, with its center at $x=x_0$, and each side parallel to either x or y, as illustrated. (The z direction is perpendicular to the page.)



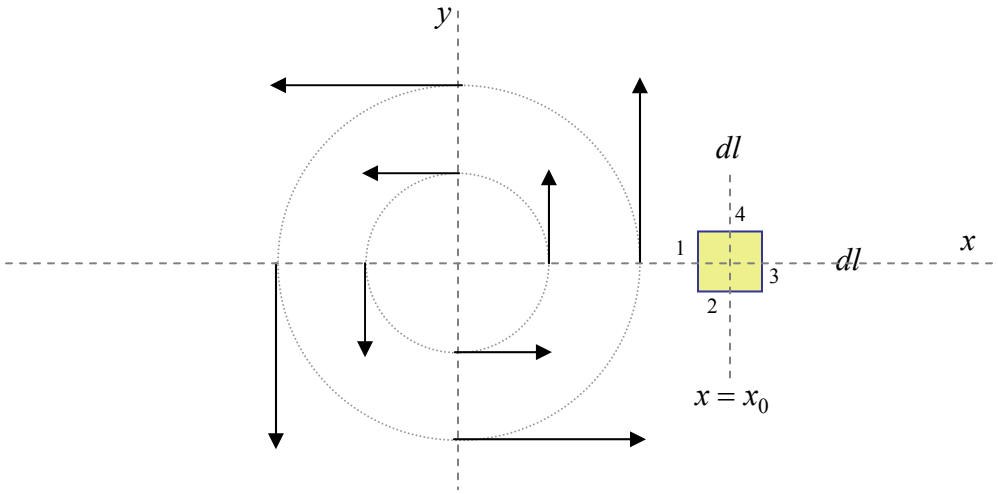
With the loop lying in the $x-y$ plane, we can use Eq. (15) to find the z component of the curl of $\mathbf{V}$ (because then the surface normal can be taken to be in the $+\hat{z}$ direction). Because $\mathbf{V}$ points in the x direction the two sides parallel to y do not contribute to the circulation. And because the top and bottom sides have tangential vectors $\hat{\mathbf{T}}_C(\mathbf{r}_C)$ pointing in opposite directions, the contributions to the circulation from these two sides cancel each other, resulting in zero net circulation for this loop. Thus $[\nabla\times\mathbf{V}(x,y,z)]_z$ is zero for this vector field.

In a similar fashion you should be able to determine the other components of $\nabla\times\mathbf{V}(\mathbf{r})$. How would you orient your loop to enable you to use Eq. (15) to calculate these other components? Do you get zero for these components as well? You can confirm that, indeed, $\nabla\times\mathbf{V}(x,y,z)=0$ by using Eq. (11) or Eq. (12). That is, all components of the curl of $\mathbf{V}(\mathbf{r})$ are, indeed, zero.

Example 2 How about the vector field

$$\mathbf{V}(x,y,z)=V_0(-y\,\hat{\mathbf{x}}+x\,\hat{\mathbf{y}})? \tag{17}$$

Let's determine whether this vector field has a nonzero curl.



The above sketch illustrates some vectors associated with this field (again drawn in the x-y plane). Does the field seem to circulate around? Because it does, we might expect the curl to be nonzero. Here we consider a small, square area sitting on the x axis at $x=x_0$ and use Eq. (15) to see what that curl is like. Here we must consider all fours sides because each side has some contribution to the curl. Assuming that the

surface normal vector is again the $\hat{z}$ direction, the fours sides contribute the following amounts to the circulation:

side 1: $-V_0(x_0 - dl/2)dl$,
side 2: $V_0(dl/2)dl$,
side 3: $V_0(x_0 + dl/2)dl$,
side 4: $V_0(dl/2)dl$.

The total circulation is thus $2V_0\,dl^2$, which tells us that $[\nabla\times\mathbf{V}(x,y,z)]_z = 2V_0$ for this field. Indeed, it is nonzero (and the same everywhere). You must think about orienting the square in three orthogonal direction in order to obtain all three components of $\nabla\times\mathbf{V}(\mathbf{r})$. You should be able to convince yourself that the other two components of $\nabla\times\mathbf{V}(\mathbf{r})$ are zero. If we so desire, we can resort to Eq. (11) or (12) to calculate the curl more directly, which produces $\nabla\times\mathbf{V}(x,y,z) = 2V_0\,\hat{\mathbf{z}}$, confirming that there is a net curl in the z direction that is the same everywhere.

IV. Some Useful Identities

We will not prove them here, but there are three identities that will be useful when we discuss Maxwell's equations. They are

$$\nabla\times(\nabla f(\mathbf{r})) = 0, \tag{18}$$

$$\nabla\cdot(\nabla\times\mathbf{V}(\mathbf{r})) = 0, \tag{19}$$

$$\nabla\times(\nabla\times\mathbf{V}(\mathbf{r})) = \nabla(\nabla\cdot\mathbf{V}(\mathbf{r})) - \nabla^2\mathbf{V}(\mathbf{r}). \tag{20}$$

We have not previously considered the Laplacian ∇^2 operating on a vector field, but looking at Eq. (4) we see that in Cartesian coordinates

$$\nabla^2\mathbf{V}(x,y,z) = \frac{\partial^2\mathbf{V}}{\partial x^2} + \frac{\partial^2\mathbf{V}}{\partial y^2} + \frac{\partial^2\mathbf{V}}{\partial z^2}, \tag{21}$$

and so $\nabla^2\mathbf{V}(\mathbf{r})$ is also a vector field.

Exercises

*__30.1__ Using Cartesian coordinates, show that
(__a__) $\nabla\times(\nabla f(x,y,z))=0$ [for any sufficiently differentiable function $f(x,y,z)$], and
(__b__) $\nabla\cdot(\nabla\times\mathbf{V}(x,y,z))=0$ [for any sufficiently differentiable vector field $\mathbf{V}(x,y,z)$].

**__30.2__ Using Cartesian coordinates, show that $\nabla\times(\nabla\times\mathbf{V}(\mathbf{r}))=\nabla(\nabla\cdot\mathbf{V}(\mathbf{r}))-\nabla^2\mathbf{V}(\mathbf{r})$ [for any sufficiently differentiable vector field $\mathbf{V}(x,y,z)$].

*__30.3__ Is Stoke's theorem applicable to a Mobius strip? Why or why not?

Maxwell's Equations

Overview and Motivation: Maxwell's (M's) equations, along with the Lorentz force law constitute essentially all of classical electricity and magnetism (E and M). One phenomenon that arises from M's equations is electromagnetic radiation, that is, electromagnetic waves. Here we introduce M's equations, discuss how they should be viewed, and see how M's equations imply the wave equation. We will look at a plane-wave solution to M's equations. We will also see that the conservation of electric charge is a direct result of Maxwell's equations.

Key Mathematics: We will gain some practice with "del" (∇) used in calculating the divergence and the curl of the electric and magnetic vector fields.

I. Maxwell's Equations

The basic Maxwell's equations are typically written, in SI units[1], as

$$\nabla \cdot \mathbf{E}(\mathbf{r},t) = \frac{\rho(\mathbf{r},t)}{\varepsilon_0}, \tag{1}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0, \tag{2}$$

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t}, \tag{3}$$

$$\nabla \times \mathbf{B}(\mathbf{r},t) = \mu_0 \, \mathbf{j}(\mathbf{r},t) + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t}. \tag{4}$$

These are coupled first-order, linear, partial differential equations for the electric and magnetic vector fields, $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$, respectively. The two constants in the equations, ε_0 and μ_0, are the fundamental constants of E and M, respectively. You probably first encountered these two constants in your introductory physics class when you studied the electric force from a point charge and the magnetic force form a long, straight wire carrying a constant current. The other two quantities in these equations are the electric charge density $\rho(\mathbf{r},t)$ and electric-charge current density $\mathbf{j}(\mathbf{r},t)$.

[1] There have been no fewer than 5 systems of units traditionally used for E and M: electrostatic (esu), electromagnetic (emu), Gaussian (cgs), Heaviside-Lorentz, and Rationalized MKSA (now known as SI). Beware when reading the literature!

So what is the meaning of Eqs. (1) – (4)? The way these equations are written you should think of the quantity on the rhs as giving rise to the quantity on the lhs of each equation. So Eq. (1) tells us that electric charge density is the source of electric field. Similarly, Eq. (2) tells us that there is no such corresponding magnetic charge density. Equation (3) tells us that a time varying magnetic field can produce an electric field, and Eq. (4) says that both an electric-charge current density and a time varying electric field can produce a magnetic field. Maxwell was actually only responsible for the last term in Eq. (4), but the term is key to E and M because without it there would be no electromagnetic radiation.

Often one considers the charge density $\rho(\mathbf{r},t)$ and current density $\mathbf{j}(\mathbf{r},t)$ to be given quantities. That is, one assumes that there is something external to the problem that controls $\rho(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ and so they are simply treated as given source terms for the equations. However, in some problems the dynamics of $\rho(\mathbf{r},t)$ and $\mathbf{j}(\mathbf{r},t)$ are determined by the fields themselves through the Lorentz force equation

$$\mathbf{F} = q\left[\mathbf{E}(\mathbf{r},t) + (\vec{v}\times\mathbf{B}(\mathbf{r},t))\right], \tag{5}$$

which describes the force on a particle with charge q and velocity v. In such cases Eqs. (1) – (5) must be solved self consistently for both the time varying fields and charge and current distributions.

II. The Conservation of Electric Charge

One of the consequences of M's equations is the conservation of electric charge. If we start with Eq. (1) and takes its time derivative, we obtain

$$\nabla\cdot\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t} = \frac{1}{\varepsilon_0}\frac{\partial\rho(\mathbf{r},t)}{\partial t}, \tag{6}$$

after switching the order of the divergence and time derivative on the lhs. Equation (4) can be rearranged as

$$\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t} = \frac{1}{\mu_0\varepsilon_0}\nabla\times\mathbf{B}(\mathbf{r},t) - \frac{1}{\varepsilon_0}\mathbf{j}(\mathbf{r},t). \tag{7}$$

Using this equation to substitute for $\partial\mathbf{E}/\partial t$ in Eq. (6) then yields

$$\nabla\cdot\left[\frac{1}{\mu_0\varepsilon_0}\nabla\times\mathbf{B}(\mathbf{r},t) - \frac{1}{\varepsilon_0}\mathbf{j}(\mathbf{r},t)\right] = \frac{1}{\varepsilon_0}\frac{\partial\rho(\mathbf{r},t)}{\partial t}. \tag{8}$$

But this simplifies considerably because $\nabla\cdot(\nabla\times\mathbf{V})=0$ for any vector field $\mathbf{V}$. Thus we have

$$\frac{\partial\rho(\mathbf{r},t)}{\partial t}+\nabla\cdot\mathbf{j}(\mathbf{r},t)=0, \tag{9}$$

the continuity equation for the charge density and the charge current density. As we discussed in an earlier lecture, the continuity equation is the local form of the statement of the conservation of the particular quantity (in this case electric charge) that corresponds to the given density and current density.

III. Wave Equations for the Electric and Magnetic Fields

As we now demonstrate, M's equations imply waves equations for both the electric and magnetic fields. To keep things simple we consider M's equations in a charge-free, current-free region of space. Then Eq. (1) – (4) become

$$\nabla\cdot\mathbf{E}(\mathbf{r},t)=0, \tag{10}$$

$$\nabla\cdot\mathbf{B}(\mathbf{r},t)=0, \tag{11}$$

$$\nabla\times\mathbf{E}(\mathbf{r},t)=-\frac{\partial\mathbf{B}(\mathbf{r},t)}{\partial t}, \tag{12}$$

$$\nabla\times\mathbf{B}(\mathbf{r},t)=\mu_0\varepsilon_0\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t}. \tag{13}$$

These are know as the homogeneous M's equations because either **E** or **B** appear linearly in every (nonzero) term in the equations. Let's derive the wave equation for the magnetic field. To do this we first take the curl of Eq. (13) to produce

$$\nabla\times\left[\nabla\times\mathbf{B}(\mathbf{r},t)\right]=\mu_0\varepsilon_0\nabla\times\frac{\partial\mathbf{E}(\mathbf{r},t)}{\partial t} \tag{14}$$

Using the identity $\nabla\times(\nabla\times\mathbf{V}(\mathbf{r}))=\nabla(\nabla\cdot\mathbf{V}(\mathbf{r}))-\nabla^2\mathbf{V}(\mathbf{r})$ on the lhs and switching the order of the curl and time derivative on the rhs then produces

$$\nabla\left[\nabla\cdot\mathbf{B}(\mathbf{r},t)\right]-\nabla^2\mathbf{B}(\mathbf{r},t)=\mu_0\varepsilon_0\frac{\partial\left[\nabla\times\mathbf{E}(\mathbf{r},t)\right]}{\partial t}. \tag{15}$$

Now using Eq. (11) to substitute for $\nabla\cdot\mathbf{B}(\mathbf{r},t)$ on the lhs and Eq. (12) to substitute for $\nabla\times\mathbf{E}(\mathbf{r},t)$ on the rhs yields

$$\nabla^2\mathbf{B}(\mathbf{r},t)=\mu_0\varepsilon_0\frac{\partial^2\mathbf{B}(\mathbf{r},t)}{\partial t^2}, \tag{16}$$

the wave equation for the magnetic field $\mathbf{B}(\mathbf{r},t)$, where the standard constant c^2 in the wave equation is equal to $1/\mu_0\varepsilon_0$. One can similarly derive the corresponding wave equation for the electric field

$$\nabla^2\mathbf{E}(\mathbf{r},t)=\mu_0\varepsilon_0\frac{\partial^2\mathbf{E}(\mathbf{r},t)}{\partial t^2}. \tag{17}$$

Notice that each of these wave equations is for a vector quantity, and so in essence each of these equations is really three wave equations, one for each component of the electric or magnetic field. Another thing to note is that while M's equations imply the wave equations for $\mathbf{E}$ and $\mathbf{B}$, the two fields are not independent. That is, all solutions to Eqs. (16) and (17) will not necessarily satisfy M's equations. Another way to think about this is that by taking a derivative (the curl) of Eq. (13) (to derive the $\mathbf{B}$-field wave equation) we lost some information originally contained in that equation.

IV. Plane Wave Solutions to M's Equations

We already know that a plane wave is one possible type of solution to the 3D wave equation. So let's assume that we have an electric field of the form

$$\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi). \tag{18}$$

Remember, the wave vector $\mathbf{k}$ points in the direction of propagation and $k\equiv|\mathbf{k}|=2\pi/\lambda$, where λ is the wavelength. Substituting Eq. (18) into Eq. (17) gives us, as usual, the dispersion relation, which in this case is $\omega=ck$ where $c=1/\sqrt{\mu_0\varepsilon_0}$ is known as the speed of light. As far as the wave equation is concerned, the dispersion relation is the only constraint that needs to be satisfied in order for Eq. (18) to be a solution.

However, M's equations put a further constraint on the electric field. Let's substitute Eq. (18) into Eq. (10). Then we obtain

$$\nabla\cdot\left[\mathbf{E}_0\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi)\right]=0 \tag{19}$$

To see what this equation implies for our plane-wave solution let's rewrite it using Cartesian coordinates,

$$\left(\frac{\partial}{\partial x}\hat{\mathbf{x}}+\frac{\partial}{\partial y}\hat{\mathbf{y}}+\frac{\partial}{\partial z}\hat{\mathbf{z}}\right)\cdot\left[\left(E_{0x}\hat{\mathbf{x}}+E_{0y}\hat{\mathbf{y}}+E_{0z}\hat{\mathbf{z}}\right)\cos\left(k_x x+k_y y+k_z z-\omega t+\phi\right)\right]=0\,. \tag{20}$$

Calculating the derivatives produces

$$\left(E_{0x}k_x+E_{0y}k_y+E_{0z}k_z\right)\sin\left(k_x x+k_y y+k_z z-\omega t+\phi\right)=0 \tag{21}$$

which can be written in coordinate-independent notation as

$$\left(\mathbf{E}_0\cdot\mathbf{k}\right)\sin\left(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi\right)=0\,. \tag{22}$$

For this to be true for all values of $\mathbf{r}$ and t, this then implies

$$\mathbf{E}_0\cdot\mathbf{k}=0\,. \tag{23}$$

So what does this tell us? Because $\mathbf{k}$ points in the direction of the wave's propagation, this tells us that the electric field must be perpendicular (or transverse) to the direction of propagation. That is, there is no longitudinal component to the electric field for a plane-wave solution to M's equations.

So what about the magnetic field? Somewhere we should have learned that electromagnetic radiation consists of both propagating electric and magnetic fields. In order to see what else M's tell us let's assume that the magnetic field associated with the electric field given by Eq. (18) is of the form

$$\mathbf{B}\left(\mathbf{r},t\right)=\mathbf{B}_0\cos\left(\mathbf{k}'\cdot\mathbf{r}-\omega' t+\phi'\right). \tag{24}$$

Let's now see what M's equations tell us about $\mathbf{B}_0$, $\mathbf{k}'$, ω', and ϕ'. As with the electric field, we can use Eq. (11) to tell us that $\mathbf{B}_0$ is also perpendicular to the direction of propagation. We can learn more by substituting Eqs. (18) and (24) into Eq. (13). After a bit of algebra and differentiation we end up with the result

$$\left(\mathbf{B}_0\times\mathbf{k}'\right)\sin\left(\mathbf{k}'\cdot\mathbf{r}-\omega' t+\phi'\right)=\frac{\omega}{c^2}\mathbf{E}_0\sin\left(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi\right), \tag{25}$$

where we have used $\mu_0\varepsilon_0=1/c^2$. For this to hold for all values of $\mathbf{r}$ and t we must have the following relationships: $\mathbf{k}'=\mathbf{k}$, $\omega'=\omega$, $\phi'=\phi$, and $\left(\mathbf{B}_0\times\mathbf{k}\right)=\left(\omega/c^2\right)\mathbf{E}_0$. The first three relationships tell us that the electric and magnetic fields have the same wavelength, frequency, and phase, and propagate in the same direction. The last relationship is a bit more interesting. The last relationship tells us that $\mathbf{E}_0$ is

perpendicular to both $\mathbf{k}$ (which we knew already) and $\mathbf{B}_0$. Thus, because both $\mathbf{E}_0$ and $\mathbf{B}_0$ are perpendicular to $\mathbf{k}$ all three vector are perpendicular to each other. Furthermore, because $(\mathbf{B}_0 \times \mathbf{k}) \| \mathbf{E}_0$ we must also have $(\mathbf{E}_0 \times \mathbf{B}_0) \| \mathbf{k}$ and $(\mathbf{k} \times \mathbf{E}_0) \| \mathbf{B}_0$. And lastly, because $\mathbf{B}_0$ and $\mathbf{k}$ are perpendicular, the relationship $(\mathbf{B}_0 \times \mathbf{k}) = (\omega/c^2)\mathbf{E}_0$ tells us that $B_0 k = (\omega/c^2)E_0$ or, because $\omega = ck$, $B_0 = E_0/c$. Thus, the magnetic field can be expressed as

$$\mathbf{B}(\mathbf{r},t) = \frac{1}{c}\left(\hat{\mathbf{k}} \times \mathbf{E}_0\right)\cos(\mathbf{k}\cdot\mathbf{r} - \omega t + \phi), \tag{26}$$

where $\hat{\mathbf{k}} = \mathbf{k}/k$. Or we can simply write, for our plane wave solution to M's equations,

$$\mathbf{B}(\mathbf{r},t) = \frac{1}{c}\hat{\mathbf{k}} \times \mathbf{E}(\vec{r},t).$$

Exercises

***31.1**. As was done in the notes for the magnetic field, derive the wave equation for the electric field.

***31.2**. The product $\mu_0\varepsilon_0$ appears in the wave equations where $1/c^2$ traditionally appears. Look up μ_0 and ε_0 and calculate $c = 1/\sqrt{\mu_0\varepsilon_0}$. What do you get?

***31.3**. Derive the dispersion relation $\omega = ck$ by substituting Eq. (18) into Eq. (17).

****31.4**. **Conditions on $\vec{E}$ and $\vec{B}$ for a plane wave**
(**a**) Substitute Eqs. (18) and (24) into Eq. (13) and derive Eq. (25).
(**b**) Substitute Eqs. (18) and (24) instead into Eq. (12) and again derive Eq. (25). This shows that in this situation the information in Eq. (12) is redundant.

****31.5**. **A traveling-wave solution to Maxwell's equations**. Show that the traveling wave fields

$$\mathbf{E}(\mathbf{r},t) = E_0\hat{\mathbf{x}}\cos(kz - \omega t) \text{ and } \mathbf{B}(\mathbf{r},t) = \frac{E_0}{c}\hat{\mathbf{y}}\cos(kz - \omega t)$$

satisfy all four homogeneous Maxwell equations.

Energy Density and the Poynting Vector

Overview and Motivation: We saw in the last lecture that electromagnetic waves are one consequence of Maxwell's (M's) equations. With electromagnetic waves, as with other waves, there is an associated energy density and energy flux. Here we introduce these electromagnetic quantities and discuss the conservation of energy in the electromagnetic fields. Further, we see how the expressions for the energy density and energy flux can be put into a form that is similar to expressions for the same quantities for waves on a string.

Key Mathematics: We will gain some more practice with the "del" operator ∇ . We will also discuss what is meant by a time-averaged quantity.

I. Energy Density and Energy-current Density in EM Waves

Recall from the last lecture the basic Maxwell's equations,

$$\nabla \cdot \mathbf{E}(\mathbf{r},t) = \frac{\rho(\mathbf{r},t)}{\varepsilon_0}, \tag{1}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0, \tag{2}$$

$$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t}, \tag{3}$$

$$\nabla \times \mathbf{B}(\mathbf{r},t) = \mu_0 \, \mathbf{j}(\mathbf{r},t) + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t}. \tag{4}$$

As we discussed last time, for $\rho(\mathbf{r},t) = 0$ and $\mathbf{j}(\mathbf{r},t) = 0$, M's equations imply the wave equation for both $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$. We know that waves transport energy. So how is the energy in an electromagnetic wave expressed? Well, you should have learned in your introductory physics course that the energy density contained in the electric field is given by[1]

$$u_{el}(\mathbf{r},t) = \frac{\varepsilon_0}{2} \mathbf{E}(\mathbf{r},t) \cdot \mathbf{E}(\mathbf{r},t) = \frac{\varepsilon_0}{2} \left[\mathbf{E}(\mathbf{r},t)\right]^2. \tag{5}$$

Typically this energy density is introduced in a discussion of the energy required to charge up a capacitor (which produces an electric field between the plates). Similarly, the energy density contained in the magnetic field is given by

[1] In keeping with standard EM notation, we use u for the energy density and $\mathbf{S}$ for the energy flux.

$$u_{mag}(\mathbf{r},t)=\frac{1}{2\mu_0}\mathbf{B}(\mathbf{r},t)\cdot\mathbf{B}(\mathbf{r},t)=\frac{1}{2\mu_0}[\mathbf{B}(\mathbf{r},t)]^2. \quad (6)$$

Typically this relationship is introduced in a discussion of the energy required to establish a current in a toroid (which produces a magnetic field inside the toroid). Notice again that the two fundamental constants of E and M, ε_0 and μ_0, appear in Eq. (5) and Eq. (6), respectively. Thus the total energy $u(\mathbf{r},t)$ contained in a region of space with both electric and magnetic fields is

$$u(\mathbf{r},t)=\frac{1}{2}\left\{\varepsilon_0[\mathbf{E}(\mathbf{r},t)]^2+\frac{1}{\mu_0}[\mathbf{B}(\mathbf{r},t)]^2\right\}. \quad (7)$$

Because $c^2=1/(\mu_0\varepsilon_0)$, this can also be written as

$$u(\mathbf{r},t)=\frac{1}{2\mu_0}\left\{\left[\frac{\mathbf{E}(\mathbf{r},t)}{c}\right]^2+[\mathbf{B}(\mathbf{r},t)]^2\right\}. \quad (8)$$

Recall, for a traveling EM wave in vacuum the electric and magnetic field amplitudes are related by $B=E/c$. Equation (8) thus shows that equal amounts of energy are contained in the electric and magnetic fields in such a wave.

What about the energy current density (also known as the energy flux)? Well, another basic fact about electromagnetic radiation (that you may or may not have learned in your introductory physics course) is that the energy flux in a particular region of space is equal to

$$\mathbf{S}(\mathbf{r},t)=\frac{1}{\mu_0}\mathbf{E}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t) \quad (9)$$

As we learned in the last lecture, the direction of propagation of an electromagnetic plane wave is in the direction of $\mathbf{E}(\mathbf{r},t)\times\mathbf{B}(\mathbf{r},t)$. As expected, Eq. (9) indicates that the energy flux points in this same direction. In E and M the energy flux is known as the **Poynting vector** (convenient because it *points* in the direction of the energy flow).

II. Continuity Equation for u and $\vec{S}$

If u and $\vec{S}$ are indeed the energy and energy-current densities, respectively, then we expect that they should be related by the continuity equation

$$\frac{\partial u(\mathbf{r},t)}{\partial t} + \nabla \cdot \mathbf{S}(\mathbf{r},t) = 0 \,. \tag{10}$$

Let's see if M's equations indeed imply Eq. (10). We first start with Eq. (8) and calculate its time derivative, which gives us

$$\frac{\partial u}{\partial t} = \frac{1}{\mu_0}\left(\frac{1}{c^2}\mathbf{E}\cdot\frac{\partial \mathbf{E}}{\partial t} + \mathbf{B}\cdot\frac{\partial \mathbf{B}}{\partial t}\right). \tag{11}$$

In deriving Eq. (11) we must remember, for example, that $\mathbf{E}^2$ is really shorthand for $\mathbf{E}\cdot\mathbf{E}$ [see Eq. (5)]. Starting with Eq. (9) we can also calculate $\nabla\cdot\mathbf{S}$, which gives us, after using the vector identity $\nabla\cdot(\mathbf{A}\times\mathbf{B}) = \mathbf{B}\cdot(\nabla\times\mathbf{A}) - \mathbf{A}\cdot(\nabla\times\mathbf{B})$,

$$\nabla\cdot\mathbf{S} = \frac{1}{\mu_0}\left[\mathbf{B}\cdot(\nabla\times\mathbf{E}) - \mathbf{E}\cdot(\nabla\times\mathbf{B})\right]. \tag{12}$$

We can now use M's Eqs. (3) and (4) to replace the curls in Eq. (12), which produces, after a bit of manipulation and the use of $\mu_0\varepsilon_0 = 1/c^2$,

$$\nabla\cdot\mathbf{S} = -\frac{1}{\mu_0}\left(\frac{1}{c^2}\mathbf{E}\cdot\frac{\partial \mathbf{E}}{\partial t} + \mathbf{B}\cdot\frac{\partial \mathbf{B}}{\partial t}\right) - \mathbf{E}\cdot\mathbf{j}. \tag{13}$$

Comparing Eqs. (11) and (13) we see that

$$\frac{\partial u}{\partial t} + \nabla\cdot\mathbf{S} = -\mathbf{E}\cdot\mathbf{j} \tag{14}$$

So what happened? Why didn't M's equations gives us Eq. (10)? Well, there is a very good reason. The energy density u and energy-current density $\mathbf{S}$ are densities associated with the fields only. But energy can also exist in the (kinetic) energy of the charge density. The term $\mathbf{E}\cdot\mathbf{j}$ is known as **Joule heating**; it expresses the rate of energy transfer to the charge carriers from the fields. This is the (spatially) local version of an equation with which you are already familiar, $P = VI$. Notice that this term only contains the electric field because the magnetic field can do no work on the charges. The term appears with a negative sign in Eq. (14) because an increase in energy of the charge carriers contributes to a decrease in energy in the fields.

Obviously, if the homogeneous M's equations apply [$\rho(\mathbf{r},t)=0$ and $\mathbf{j}(\mathbf{r},t)=0$], then Eq. (10), the standard continuity equation is indeed valid.

III. The densities u and $\mathbf{S}$ for an EM Plane Wave

In the last lecture we looked at the plane-wave solution

$$\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi) \tag{15}$$

$$\mathbf{B}(\mathbf{r},t)=\frac{1}{c}(\hat{\mathbf{k}}\times\mathbf{E}_0)\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi) \tag{16}$$

to the homogeneous Maxwell's equations. Let's calculate u and $\vec{S}$ for these fields. Substituting Eqs. (15) and (16) into Eqs. (8) and (9) produces

$$u(\mathbf{r},t)=\frac{1}{c}\sqrt{\frac{\varepsilon_0}{\mu_0}}[E_0\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi)]^2, \tag{17}$$

and

$$\mathbf{S}(\mathbf{r},t)=\sqrt{\frac{\varepsilon_0}{\mu_0}}[E_0\cos(\mathbf{k}\cdot\mathbf{r}-\omega t+\phi)]^2\hat{\mathbf{k}}, \tag{18}$$

respectively. Comparing Eqs. (17) and (18) we see that

$$\mathbf{S}(\mathbf{r},t)=c\,u(\mathbf{r},t)\hat{\mathbf{k}}. \tag{19}$$

The agrees with the general expectation for a traveling wave that the energy current flux $\mathbf{j}_\varepsilon(\mathbf{r},t)$ is related to its associated energy density $\rho_\varepsilon(\mathbf{r},t)$ via $\mathbf{j}_\varepsilon(\mathbf{r},t)=\rho_\varepsilon(\mathbf{r},t)\mathbf{v}$, where $\mathbf{v}$ is the velocity of $\rho_\varepsilon(\mathbf{r},t)$.

The Poynting vector expressed in Eq. (18) is a space and time dependent quantity. Often, however, often we are more interested in the time-averaged value of this quantity. In general, the time-averaged value of a periodic function with period T is given by

$$\langle A(t)\rangle_t=\frac{1}{T}\int_0^T A(t)dt. \tag{20}$$

With this definition the time-averaged value of $\mathbf{S}$ is

$$\langle \mathbf{S}(t) \rangle_t = E_0^2 \sqrt{\frac{\varepsilon_0}{\mu_0}} \hat{\mathbf{k}} \left\{ \frac{\omega}{2\pi} \int_0^{\omega/2\pi} [\cos(\mathbf{k}\cdot\mathbf{r} - \omega t + \phi)]^2 \, dt \right\} \tag{21}$$

Because the average value of any harmonic function squared is simply $1/2$, we have

$$\langle \mathbf{S}(t) \rangle_t = \frac{E_0^2}{2} \sqrt{\frac{\varepsilon_0}{\mu_0}} \hat{\mathbf{k}}. \tag{22}$$

On last remark about $\langle \mathbf{S}(\mathbf{r},t) \rangle_t$. In the optics world $\langle \mathbf{S}(\mathbf{r},t) \rangle_t$ is known as the **intensity** associated with the electromagnetic wave. Its dot product with a normal vector to some surface gives the average power per unit area incident on that surface.

IV. An Analogy Between Mechanical and EM Waves

We previously studied the energy contained in mechanical waves. In particular, we looked at transverse waves on a string, which have an energy density and energy-current density that were essentially expressed as

$$\rho_\varepsilon(x,t) = \frac{\tau}{2} \left\{ \left[\frac{1}{c} \frac{\partial q(x,t)}{\partial t} \right]^2 + \left[\frac{\partial q(x,t)}{\partial x} \right]^2 \right\}, \tag{23}$$

$$j_\varepsilon(x,t) = -\tau \left[\frac{\partial q(x,t)}{\partial t} \right] \left[\frac{\partial q(x,t)}{\partial x} \right]. \tag{24}$$

As they stand, these equations do not look particularly like Eqs. (8) and (9) for the corresponding electromagnetic quantities.

The mechanical-waves expressions are written in terms of derivatives of the displacement while the electromagnetic quantities are written in terms of the fields. However, in the theory of electricity and magnetism we can introduce a quantity known as the vector potential $\mathbf{A}(\mathbf{r},t)$ that, in the absence of $\rho(\vec{r},t)$ and $\mathbf{j}(\mathbf{r},t)$, can be defined such that it is related to the electric and magnetic fields via

$$\mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t} \tag{25}$$

and

$$\mathbf{B}(\mathbf{r},t)=\nabla\times\mathbf{A}(\mathbf{r},t). \tag{26}$$

Substituting these expressions into Eqs. (8) and (9) then gives us two equations that now look quite similar to Eqs. (23) and (24),

$$u(\mathbf{r},t)=\frac{1}{2\mu_0}\left\{\left[\frac{1}{c}\frac{\partial\mathbf{A}(\mathbf{r},t)}{\partial t}\right]^2+\left[\nabla\times\mathbf{A}(\mathbf{r},t)\right]^2\right\}, \tag{27}$$

$$\mathbf{S}(\mathbf{r},t)=-\frac{1}{\mu_0}\left(\frac{\partial\mathbf{A}(\mathbf{r},t)}{\partial t}\times\left[\nabla\times\mathbf{A}(\mathbf{r},t)\right]\right). \tag{28}$$

For a more exact analogy, let's go back to Eqs. (15) and (16), the plane-wave solution to M's equations. Let's simplify things by choosing the coordinate system so that $\mathbf{k}$ points in the $+x$ direction, $\mathbf{E}_0$ points along the $+y$ direction, which leaves $\mathbf{B}_0$ to point along the $+z$ direction. The electric and magnetic fields for the plane wave can then be written as

$$\mathbf{E}(x,t)=E_0\hat{\mathbf{y}}\cos(kx-\omega t+\phi), \tag{29}$$

$$\mathbf{B}(x,t)=\frac{E_0}{c}\hat{\mathbf{z}}\cos(kx-\omega t+\phi). \tag{30}$$

These two fields are consistent with the vector potential

$$\mathbf{A}(x,t)=\frac{E_0}{\omega}\hat{\mathbf{y}}\sin(kx-\omega t+\phi)=A_y(x,t)\hat{\mathbf{y}}. \tag{31}$$

With this vector potential the time derivative and curl of $\mathbf{A}$ simplify to $\partial\mathbf{A}/\partial t=(\partial A_y/\partial t)\hat{\mathbf{y}}$ and $\nabla\times\mathbf{A}=(\partial A_y/\partial x)\hat{\mathbf{z}}$ so that

$$\left(\frac{\partial\mathbf{A}}{\partial t}\right)^2=\left(\frac{\partial A_y}{\partial t}\right)^2, \tag{32}$$

$$(\nabla\times\mathbf{A})^2=\left(\frac{\partial A_y}{\partial x}\right)^2, \tag{33}$$

and

$$\frac{\partial \mathbf{A}}{\partial t}\times\left(\nabla\times\mathbf{A}\right)=\frac{\partial A_y}{\partial t}\frac{\partial A_y}{\partial x}\hat{\mathbf{x}}\,. \tag{34}$$

With these last three expressions we can express u and $\vec{S}$ for our plane wave solution [Eqs. (31) and (32)] as

$$u(x,t)=\frac{1}{2\mu_0}\left\{\left[\frac{1}{c}\frac{\partial A_y}{\partial t}\right]^2+\left[\frac{\partial A_y}{\partial x}\right]^2\right\}, \tag{35}$$

$$\mathbf{S}(x,t)=-\frac{1}{\mu_0}\frac{\partial A_y}{\partial t}\frac{\partial A_y}{\partial x}\hat{\mathbf{x}}\,. \tag{36}$$

These expression are now essentially identical to Eqs. (23) and (24), the analogous expressions for mechanical waves on a string if the following correspondences are made: $q\leftrightarrow A_y$ and $\tau\leftrightarrow 1/\mu_0$.

Exercises

***32.1** Show that Eqs. (29) and (30) follow from Eq. (31).

****32.2 A traveling-wave solution to Maxwell's equations**. Consider the electric field $\mathbf{E}(r,t)=E_0\hat{\mathbf{x}}\cos(kz-kct)$

(**a**) What is the corresponding magnetic field?
(**b**) Calculate the energy density $u(z,t)$ associated with each of these fields.
(**c**) Calculate the Poynting vector $\mathbf{S}(z,t)$ associated with these fields.
(**d**) Show that $u(z,t)$and $\mathbf{S}(z,t)$satisfy the appropriate continuity equation.

***32.3** Show in the absence of charge and current densities that – in general – the vector potential $\mathbf{A}(\mathbf{r},t)$ satisfies the wave equation. In addition to equations in the notes, you will need to use the fact that the vector potential satisfies $\nabla\cdot\mathbf{A}=0$.