

# Brian Blais' Homemade Guide to the Diffusion Equation

## 1 Introduction

One can approach the solution of a differential equation in several ways. In this document I will outline one way to solve a differential equation, and use as an example of this the diffusion equation. The methods described can be used for many differential equations such as the wave equation and Schrödinger's equation.

The diffusion equation is

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} = A \nabla^2 \rho(\mathbf{x}, t) \quad (1.1)$$

What we are looking for are functions  $\rho(\mathbf{x}, t)$  such that, when they are placed in Equation 1.1 the equation holds true. There may be many such functions (such as  $\rho(\mathbf{x}, t) = 0$ ), but we are only interested in the physically meaningful or interesting (non trivial) solutions.

A rule of thumb for solving physics problems is to know the answer before you start, otherwise you don't know if you are doing something incorrectly. Well, we won't be able to know the complete solution without doing the math, but we can try to figure out what kinds of solutions we expect because we happen to know the physics behind it. The diffusion equation is used to describe the spreading out of some quantity of *stuff*. That *stuff* could be temperature spreading through a medium or a drop of food coloring spreading in a glass of milk, for example. The  $\rho$  in Equation 1.1 is the density of the quantity that we are talking about, so we would expect that the curve of  $\rho(\mathbf{x}, t)$  would flatten out as time goes on, representing the thinning out of the substance over space. We expect, then, that any solution must decay in time. Notice also that the  $\nabla^2$  is like the *curvature* of the function  $\rho(\mathbf{x}, t)$  (in one dimension it would be  $\partial^2/\partial x^2$ ) which suggests that the diffusion equation is flattening out the density function by making functions of high curvature change faster than ones of lower curvature.

Now that we understand the physics behind the equation, and have a *feel* for what it is trying to tell us, we are ready to find the solutions of it. We will focus primarily on the one dimensional case, for clarity, and then move onto higher dimensional forms later.

## 2 One Dimensional Solution

We begin with the one dimensional form of the diffusion equation

$$\frac{\partial \rho(x, t)}{\partial t} = A \frac{\partial^2 \rho(x, t)}{\partial x^2} \quad (2.2)$$

To solve this we will assume that the function we are looking for is *separable*, that is it can be separated into a purely time dependent part and a purely position dependant part.

$$\rho(x, t) = F(t)G(x)$$

Plugging this into Equation 2.2 we can get the form of the solution.

$$\begin{aligned} \frac{\partial F(t)G(x)}{\partial t} &= A \frac{\partial^2 F(t)G(x)}{\partial x^2} \\ G(x) \frac{dF(t)}{dt} &= AF(t) \frac{d^2 G(x)}{dx^2} \\ \frac{1}{F(t)} \frac{dF(t)}{dt} &= A \frac{1}{G(x)} \frac{d^2 G(x)}{dx^2} \end{aligned}$$

We now notice that left hand side of our result is purely a function of time, and the right hand side of our result is purely a function of position. The only way for a function of time to be equal to a function of position is for them both to be constant. Looking at the units in the equation allows us to say that the constant has units of 1/second. With a little bit of foresight, we will choose the constant to be negative (we will see why later), and equal to  $-1/\tau$ . With this assignment, we can easily get the forms of  $F(t)$  and  $G(x)$ .

$$\begin{aligned} \frac{1}{F(t)} \frac{dF(t)}{dt} &\equiv -\frac{1}{\tau} \\ \frac{dF(t)}{dt} &= -\frac{F(t)}{\tau} \\ F(t) &= F_o e^{-t/\tau} \\ A \frac{1}{G(x)} \frac{d^2 G(x)}{dx^2} &\equiv -\frac{1}{\tau} \\ \frac{d^2 G(x)}{dx^2} &= -\frac{G(x)}{A\tau} \\ G(x) &= G_o e^{-ix/\sqrt{A\tau}} \end{aligned}$$

If we define  $k \equiv 1/\sqrt{A\tau}$ , then our final solution looks like

$$\rho(x, t) = G(x)F(t) = \rho_o e^{-ikx} e^{-k^2 At} \quad (2.3)$$

### 3 Discussion of the Solution

Now that we have a solution, we have to ask ourselves what it means, and whether it makes physical sense. First of all we notice that  $F(t)$  which governs our time dependence does indeed have a decay in time, as we expect. If we had chosen our constant about to be  $+1/\tau$  we would have had exponentially *growing* solutions which still would satisfy the diffusion equation, but would be unphysical (they would violate conservation of energy).

Looking at the form of  $G(x)$  we notice that it is a simple oscillatory solution (recall Euler's formula:  $e^{i\phi} = \cos(\phi) + i \sin(\phi)$ ). Sines and cosines by themselves would also satisfy the equation for  $G(x)$ , but we choose to use exponentials because they are easiest to use. Notice, now, that for a given frequency ( $k \propto$  frequency) there is a specific decay time ( $1/k^2 A$ ), so if we had a density function that started out like a sine wave in position it would have a specific decay time.

Of course, in general, we do not start out with a oscillatory density function. We usually start out with something that is fairly peaked (dense) at a certain position. What do we do then? We can represent any function as a sum of sines and cosines of different frequency and amplitude through Fourier analysis, and then each sine or cosine has its own characteristic decay time. Because each sine in the sum decays at a different rate, the density function changes form drastically over time. The higher frequencies get damped out much more quickly, as seen from the  $k^2$  in the time exponential, as the diffusion process acts to flatten out the density function.

Now we have a recipe for solving our problem given some particular initial density function. First we take our initial density function ( $\rho(x, 0)$ ) which is a function of position, and find out what frequencies it is made of. Essentially we will be getting the density function as a function of  $k$  (as opposed to  $x$ ) at time  $t = 0$ . We will call this function  $\tilde{\rho}(k, 0)$ . Now for each  $k$  there is a particular exponential decay in time, so our full (time *dependent*) density function (still a function of  $k$ ) is

$$\tilde{\rho}(k, t) = \tilde{\rho}(k, 0) e^{-k^2 At}$$

We now need to transform back to a function of position to get the time dependent density function we are after:  $\rho(x, t)$ . It sounds like a pretty straightforward recipe, but along the way we often run into integrals we cannot directly solve and we must resort to approximation methods, or numerical techniques. I will go through the absolute simplest (non trivial) example one can solve without such techniques.

## 4 An Example: Gaussian Initial Condition

We are going to use as an initial density function a Gaussian function

$$\rho(x, 0) = \rho_0 e^{-x^2/L^2} \quad (4.4)$$

A graph of Equation 4.4 is shown in Figure 1. One can see that it is peaked at the origin, and can be thought of physically as a drop of food coloring in a glass of milk. At the moment the food coloring is dropped it has most of its density in the center and none far away from it. As time goes on, we expect the density curve to spread out and become flatter, as the food coloring reaches a more uniform density across the surface.

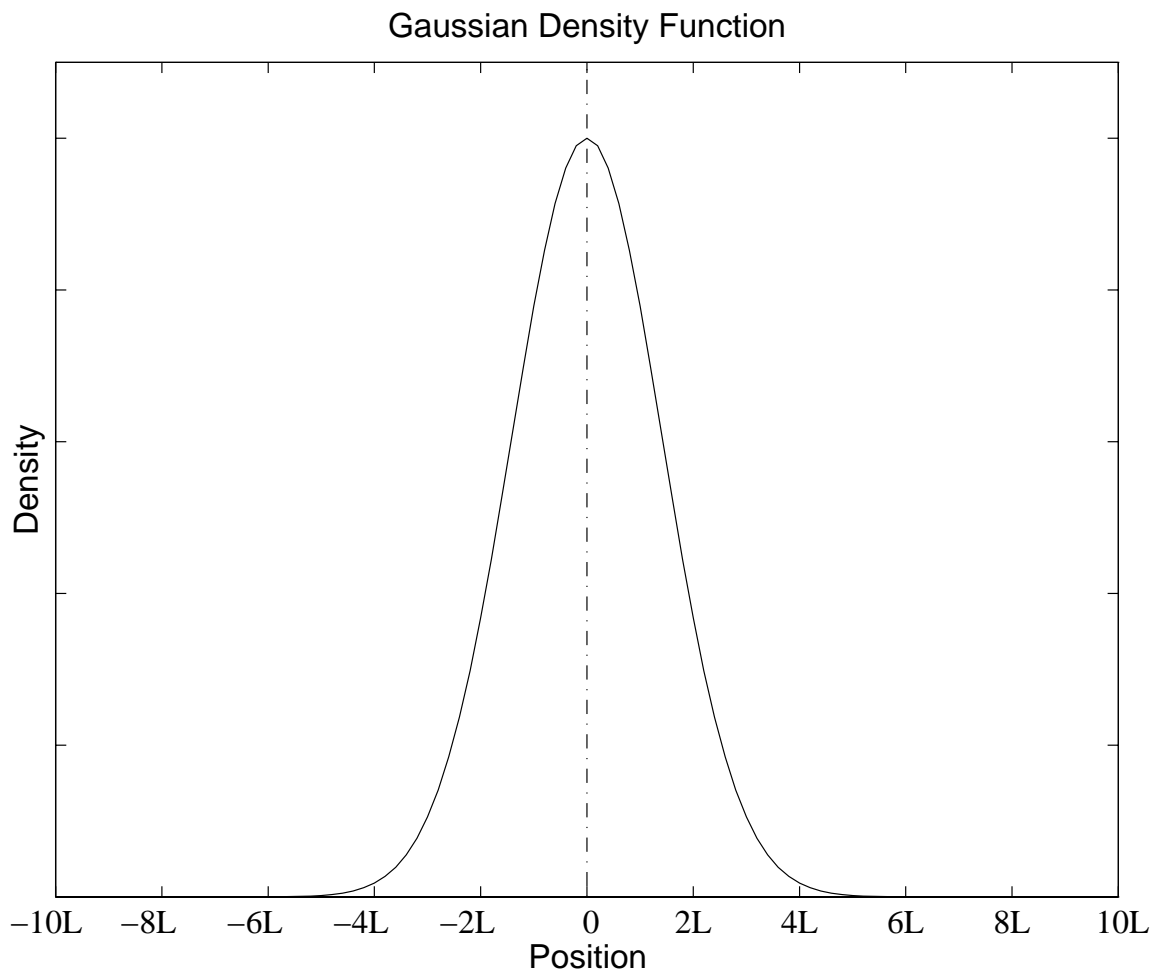


Figure 1: Gaussian Density Function

Following our recipe, we can now approach a full solution of our problem for this choice of initial

conditions.

### $\tilde{\rho}(k, 0)$ : Moving into frequency space

The first step in our recipe is to break down the function which describes our initial condition into its constituent frequencies. Our solution for the diffusion equation gives us the time dependent behavior for functions of frequency, not position. The method for doing this is a *Fourier Transform*, more specifically evaluating the following integral

$$\begin{aligned}\tilde{\rho}(k, 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \rho(x, 0) e^{ikx} dx \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \rho_0 e^{-x^2/L^2} e^{ikx} dx\end{aligned}\quad (4.5)$$

One could always just look up this integral in a big book of integrals, but if one were to find oneself on the beach and in desperate need of doing this integral it is a good idea to know how to do it. For this we need to talk a little bit about solving Gaussian integrals.

### Aside on Gaussian Integrals

The basic Gaussian integral is

$$I = \int_{-\infty}^{+\infty} e^{-ax^2} dx \quad (4.6)$$

In order to solve this, let's first consider  $I^2$  which is

$$I^2 = \int_{-\infty}^{+\infty} e^{-ax^2} dx \int_{-\infty}^{+\infty} e^{-ay^2} dy = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} e^{-a(x^2+y^2)} dx dy \quad (4.7)$$

The reason for introducing another integration variable ( $y$ ) can be understood if one thinks of the integral as a sum, so the product of two sums is the sum of all of the different products of the individual elements in the sum. Thus the double integral. We now notice that if we were to work in polar coordinates,  $x^2 + y^2$  would become  $r^2$  and the infinitesimal area  $dx dy$  would become  $r dr d\phi$ , and our integral would take on a much easier form

$$\begin{aligned}u &\equiv ar^2 \\ du = 2ardr &\Rightarrow \frac{du}{2a} = r dr \\ I^2 &= \int_0^\infty e^{-ar^2} r dr \int_0^{2\pi} d\phi \\ &= 2\pi \int_0^\infty e^{-u} du \frac{1}{2a} \\ &= \frac{-\pi}{a} e^{-u} \Big|_0^\infty \\ &= 0 - \frac{-\pi}{a} \\ &= \frac{\pi}{a} \\ I &= \sqrt{\frac{\pi}{a}}\end{aligned}\quad (4.8)$$

In order to fully tackle our diffusion problem we need to deal with a more general form the the Gaussian integral

$$I = \int_{-\infty}^{+\infty} e^{-(ax^2+bx)} dx \quad (4.9)$$

Now we have to beat Equation 4.9 into the form of Equation 4.6 so we can use the solution we arrived at earlier. To do this we complete the square in the exponent

$$\begin{aligned} I &= \int_{-\infty}^{+\infty} e^{-(ax^2+bx)} dx \\ &= \int_{-\infty}^{+\infty} e^{-(ax^2+bx+\frac{b^2}{4a}-\frac{b^2}{4a})} dx \\ &= \int_{-\infty}^{+\infty} e^{-(\sqrt{a}x+\frac{b}{2\sqrt{a}})^2+\frac{b^2}{4a}} dx \\ &= e^{\frac{b^2}{4a}} \int_{-\infty}^{+\infty} e^{-u^2} du \frac{1}{\sqrt{a}} \\ (\text{Using Equation 4.8}) &= e^{\frac{b^2}{4a}} \sqrt{\frac{\pi}{a}} \end{aligned} \quad (4.10)$$

Here we conclude our aside on Gaussian integrals. We will use the results of this shortly to solve the problem at hand.

### Continuing with the problem

Before our aside, we were confronted with the integral in Equation 4.5. Now we can use our solution in Equation 4.10 to easily compute this integral.

$$\begin{aligned} \tilde{\rho}(k, 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \rho_o e^{-(x^2/L^2-ikx)} dx \\ &= \frac{\rho_o}{\sqrt{2\pi}} e^{\frac{(-ik)^2}{4(1/L^2)}} \sqrt{\frac{\pi}{1/L^2}} \\ &= \frac{\rho_o L}{\sqrt{2}} e^{\frac{-k^2 L^2}{4}} \end{aligned} \quad (4.11)$$

### $\tilde{\rho}(k, t)$ : Adding time dependence

Adding the time dependence to the initial condition, which is stated in frequency space (sometimes called  $k$ -space because  $k \propto \text{frequency}$ ) is really quite trivial. All we need to do is tack on the time dependent piece we found from the diffusion equation.

$$\begin{aligned} \tilde{\rho}(k, t) &= \tilde{\rho}(k, 0) e^{-k^2 At} \\ &= \frac{\rho_o L}{\sqrt{2}} e^{\frac{-k^2 L^2}{4}} e^{-k^2 At} \\ &= \frac{\rho_o L}{\sqrt{2}} e^{-k^2 (\frac{L^2}{4} + At)} \end{aligned} \quad (4.12)$$

### $\rho(x, t)$ : Back to position space

Our final step is to transform Equation 4.12 into position space, making it a function of  $x$  as opposed to a function of  $k$ . In order to transform back we must do another Fourier integral (this time with a

minus sign in the exponent) and use the gaussian integral solution in Equation 4.10 to obtain a final solution to our problem.

$$\begin{aligned}
\rho(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{\rho}(k, t) e^{-ikx} dx \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{\rho_o L}{\sqrt{2}} e^{-k^2(\frac{L^2}{4} + At)} e^{-ikx} dx \\
&= \frac{\rho_o L}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-\left(\left(\frac{L^2}{4} + At\right)k^2 + (ix)k\right)} dx \\
&= \frac{\rho_o L}{2\sqrt{\pi}} e^{\frac{(ix)^2}{4(L^2/4 + At)}} \frac{\sqrt{\pi}}{(L^2/4 + At)^{\frac{1}{2}}} \\
&= \rho_o \frac{L}{2(L^2/4 + At)^{\frac{1}{2}}} e^{\frac{-x^2}{4(L^2/4 + At)}}
\end{aligned} \tag{4.13}$$

Now that we have an answer to our problem, we have to check to see whether it makes sense. There are 3 quick ways to check the answer: i) make sure the units are all correct, ii) see whether it gives our initial condition when we set  $t = 0$ , and iii) see whether it conforms to our expectation for  $t \rightarrow \infty$ .

I have written Equation 4.13 in the way that I have so that checking units will be easy.  $\rho(x, t)$  has the units of density, and so does  $\rho_o$ . Everything else should then have no dimensions, which we can easily verify. From the original diffusion equation (Equation 1.1) we can see that the constant  $A$  has the units of  $(length)^2/(second)$ , so  $(L^2/4 + At)$  has the units of  $(length)^2$ .  $x^2/4(L^2/4 + At)$  is then dimensionless, as it must be to exist in the exponent, and outside of the exponent  $L/\sqrt{L^2/4 + At}$  is also dimensionless so the units of our solution are correct.

One can clearly see that if we plug  $t = 0$  into Equation 4.13 that we obtain our initial condition seen in Equation 4.4. For large  $t$  we see that the  $1/\sqrt{t}$  out front squashes the density function, and conforms with our expectations. A graph of Equation 4.13 can be seen in Figure 2. We are now ready to discuss two dimensional and three dimensional solutions.

## 5 Moving into Higher Dimensions

In order to solve for higher dimensions, all we need to do is choose which coordinate system to use, write the Laplacian ( $\nabla^2$ ) in that coordinate system and solve using the same techniques as described above. For example, in two dimensional Cartesian coordinates the diffusion equation becomes

$$\frac{\partial \rho(x, y, t)}{\partial t} = A \nabla^2 \rho(x, y, t) = A \frac{\partial^2 \rho(x, y, t)}{\partial x^2} + A \frac{\partial^2 \rho(x, y, t)}{\partial y^2} \tag{5.14}$$

Using the separation of variables technique on this equation, this time separating into  $F(t)$ ,  $G(x)$ , and  $H(y)$ , one can easily obtain the solution for  $\rho(x, y, t)$ .

$$\rho(x, y, t) = \rho_o e^{-ik_x x} e^{-ik_y y} e^{-(k_x^2 + k_y^2)At} \tag{5.15}$$

Again we can follow the recipe for general initial conditions, but this time we have to do Fourier Transforms with respect to  $k_x$  and  $k_y$ . Otherwise the recipe goes unchanged. Unfortunately many physical systems do not have Cartesian symmetry, so we would be making our life much more difficult by performing all of the integrals in Cartesian coordinates. I will outline the solution for the two

## Gaussian Dispensing in Time

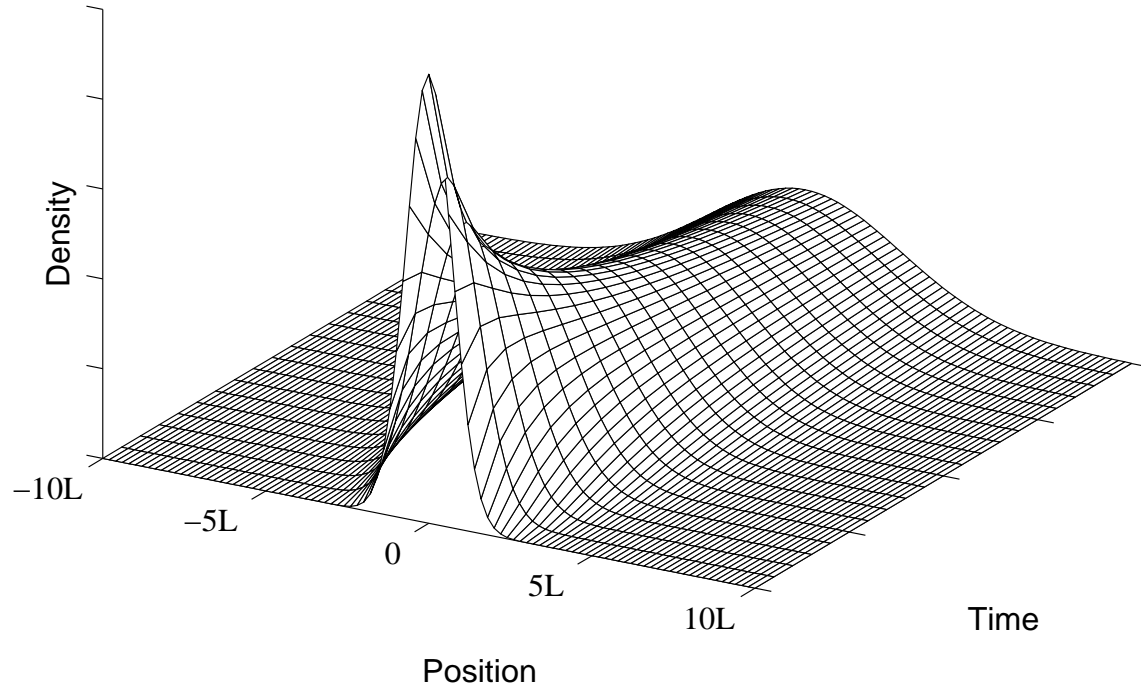


Figure 2: Gaussian Density Function Evolving in Time

dimensional polar coordinate situation, which is one that is useful for many physical applications. Our diffusion equation in polar coordinates is

$$\begin{aligned} \frac{\partial \rho(r, \phi, t)}{\partial t} &= A \nabla^2 \rho(r, \phi, t) \\ &= \frac{A}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \rho(r, \phi, t)}{\partial r} \right) + \frac{A}{r^2} \frac{\partial^2 \rho(r, \phi, t)}{\partial \phi^2} \end{aligned} \quad (5.16)$$

We now separate variables and solve each piece one at a time as we did before.

$$\begin{aligned} \rho(r, \phi, t) &= R(r)\Phi(\phi)F(t) \\ \frac{1}{F} \frac{dF}{dt} &= \frac{A}{R} \left( \frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} \right) + \frac{A}{r^2} \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \\ &\equiv -\frac{1}{\tau} \\ \frac{1}{F} \frac{dF}{dt} &= -\frac{1}{\tau} \\ \frac{dF}{dt} &= -\frac{F}{\tau} \end{aligned}$$

$$\begin{aligned}
F(t) &= F_o e^{-t/\tau} \\
-\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} &= \frac{r^2}{R} \frac{d^2 R}{dr^2} + \frac{r}{R} \frac{dR}{dr} + \frac{r^2}{A\tau} \\
&\equiv m^2 \\
-\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} &= m^2 \\
\frac{d^2 \Phi}{d\phi^2} &= -m^2 \Phi \\
\Phi(\phi) &= \Phi_o e^{im\phi} \\
\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + \left( \frac{1}{A\tau} - \frac{m^2}{r^2} \right) R &= 0 \\
\frac{d^2 R}{dr^2} + \frac{1}{r} \frac{dR}{dr} + \left( k^2 - \frac{m^2}{r^2} \right) R &= 0 \\
R(r) &= R_o J_m(r/\sqrt{At}) \\
&= R_o J_m(kr)
\end{aligned}$$

where  $J_m(kr)$  are known as *Bessel functions*, and satisfy the above differential equation. One can obtain series representations of these functions, and one can look up different properties of them in a book of integrals. One can represent other functions in terms of these, so our Fourier recipe that we used earlier (with sines and cosines) work with Bessel functions, only the forms are slightly more complicated. Our two dimensional polar solution to the diffusion equation is

$$\rho(r, \phi, t) = \rho_o J_m(kr) e^{im\phi} e^{-k^2 At} \quad (5.17)$$

One can perform similar derivations for the three dimensional case, but I will leave that to the interested reader. We have seen that the problem becomes much more difficult for higher dimensions, but luckily we can use symmetry to reduce our work in many situations. The methods described here can be used to solve many differential equations, so more information about them can be found in texts on quantum mechanics, fluid mechanics, or wave mechanics.