1.3: Classical Description of a Wave on a String

The mathematics used in solving quantum mechanical problems follow be the same basic process for each of the different problems we will examine. In this section, those mathematics will be developed in order to describe a (hopefully) familiar problem in classical physics.

Consider a wave on a string of length a which is fixed at both ends ($x = 0$ and $x = a$.) Classical physics tells us that the wave will obey the following condition

$$\frac{\partial^2}{\partial x^2}\varphi\left(x,t\right) = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}\varphi(x,t)$$

where $\phi(x,t)$ gives the displacement of the string from equilibrium at position x and time t.

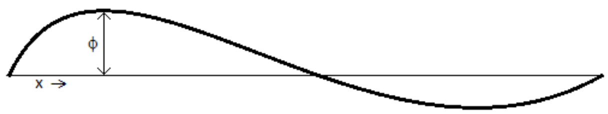

Figure 1.3.1

To solve this second order partial differential equation, we separate the function into the product of a function which deals only in position and one which deals only in time.

$$\text{Let } \phi(x,t) = X(x)T(t)$$

Substituting this form in to the equation above and gathering spatial variables on one side and time variables on the other, we get

$$\frac{\partial^2}{\partial x^2}\,X(x)T(t) = \frac{1}{v^2}\frac{\partial^2}{\partial t^2}X(x)T(t)$$

$$T(t)\frac{d^2}{dx^2}\,X(x) = \frac{X(x)}{v^2}\frac{d^2}{dt^2}T(t)$$

Notice how the partial derivatives become total derivatives since the functions on which they operate depend only on the variables in the given derivative operators. Now dividing both sides by $X(x)T(t)$ yields

$$\frac{1}{X(x)}\frac{d^2}{dx^2}X(x) = \frac{1}{v^2T(t)}\frac{d^2}{dt^2}T(t)$$

The only way this can be true is if each side is equal to a constant. Since I already know the answer, I am going to cheat and let that constant be $-k^2$ since this will avoid imaginary numbers in the solution. So now we generate two separated second order differential equations:

$$\frac{d^2}{dx^2}X(x) = -k^2X(x)$$

$$\frac{d^2}{dt^2}T(t) \;=\; -v^2k^2T(t)$$

These two equations are of a special type called **eigenvalue-eigenfunction relationship**. In these type of relationships, the operator (in this case a second derivative) operates on a function, yielding the same function multiplied by a constant. These type of relationships exist throughout quantum mechanics.

The Spatial Solutions

Let's consider only the spatial portion for the time being. Being a second order normal differential equation, there will be two linearly independent functions $X(x)$ which satisfy the equation. Two fairly obvious choices to this **eigenvalue-eigenfunction** problem are

$$X(x) = \sin(kx) \text{ and } X(x) = \cos(kx)$$

As mathematics would have it, any linear combination of these two solutions will also be a solution. Thus, it is convenient to write a general solution that is a linear combination of the two linearly independent functions.

$$X(x) = A\sin(kx) + B\cos(kx)$$

We will now employ the boundary conditions to find values for the variables A, B and k. The boundary conditions are that the string is fixed at both ends. Thus we know that $X(0) = 0$ and $X(a) = 0$

Using the first condition, we see that

$$\begin{aligned} X(0) &= A\sin(k \cdot 0) + B\cos(k \cdot 0) \\ &= 0 + B \\ &= 0 \end{aligned}$$

This can only be true if $B = 0$ since the cosine term will give a non-zero contribution for any non-zero value of B implying that the string is displaced from its fixed position, which it can not be since it is fixed at that position. For the remainder of the solution to this problem, the cosine term will be neglected since it must vanish in order to ensure that $X(0) = 0$.

The second condition is that $X(a) = 0$. This requires that

$$X(a) = A\sin(k \cdot a) = 0$$

One way of making this true is if $A = 0$. This is known as a trivial solution since it implies that $X(x)$ is zero for any value of x (meaning the string is never displaced from equilibrium at any point.) Many problems have trivial solutions, but these are generally ignored as they add no useful insight into the physical behavior of a system.

To get the non-trivial solutions, it is useful to know when $\sin(\alpha) = 0$. This will be true if α is an integral multiple of π. Thus,

$$k \cdot a = n\pi \quad n = 1, 2, 3\ldots$$

Or

$$k = \frac{n\pi}{a} \quad n = 1, 2, 3\ldots$$

Another way to think of this is that the second condition ($X(a) = 0$) can only be met if the length of the string (a) is a half integral multiple of the wavelength of the sine function.

Since there are several (an infinite number, really) possible values of n, the solution implies an infinite number of functions as solutions. Further, there is no reason to expect that A needs to be the same for each value of n.

$$X_n(x) = A_n \sin\left(\frac{n\pi x}{a}\right)$$
$$n = 1, 2, 3...$$

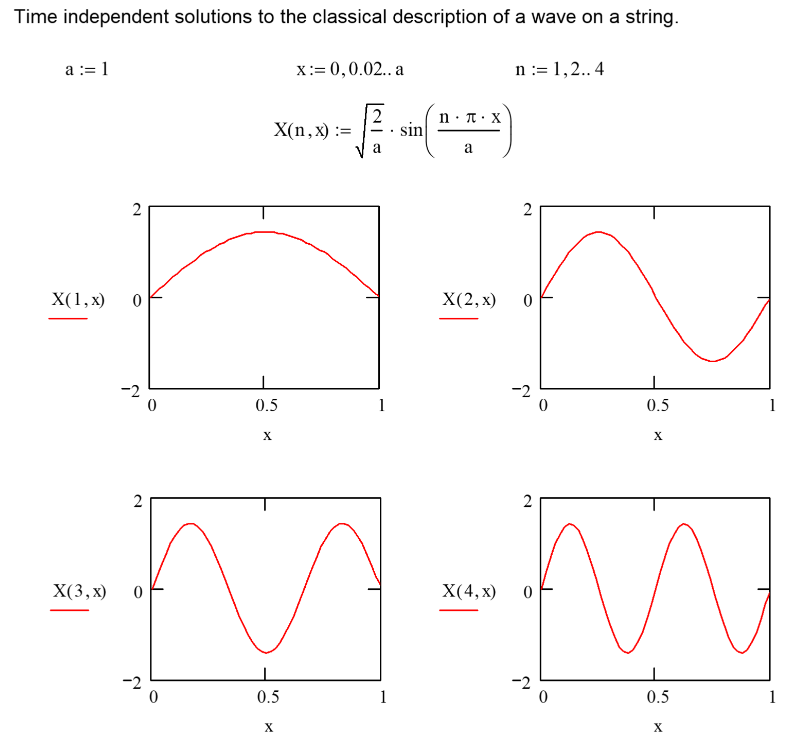

Figure 1.3.2

Since we have only two boundary conditions, we can only determine two of the unknown quantities. The last one, A_n, will govern the amplitude of the particular function. A large value implies that the string will be displaced a large amount from its equilibrium position. Thus, there may be a different value of A_n for each value of n (which is why the subscript is included.) For the time being though, let's leave A_n as a symbolic variable and evaluate it later.

Before continuing with the time portion of the problem, let's note some interesting properties of the solutions of the spatial portion. The functions $X_n(x)$ are called the "normal modes" of vibration for the string (sometimes they are called the time-independent modes.) That means that a string which is prepared to vibrate with the displacements given by one of the functions $X_n(x)$ will have a standing wave. In other words, the nodes (the places along the string where the string does not move or $X_n(x) = 0$) are stationary.

Further, the functions $X_n(x)$ form an orthogonal set. This implies that

$$\int X_n(x) X_m(x)\, dx = A_n A_m \int \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = A_n A_m \delta_{nm}$$

To prove this, it is useful to consider the following result that can be found in a standard table of integrals.

$$\int \sin(\alpha x) \sin(\beta x) d\tau = \frac{\sin[(\alpha-\beta)x]}{2(\alpha-\beta)} - \frac{\sin[(\alpha+\beta)x]}{2(\alpha+\beta)} \quad (\alpha \neq \beta)$$

Substitution into the above expression yields

$$\begin{aligned} A_n A_m \int_{x=0}^{x=a} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) x &= A_n A_m \left[\frac{\sin\left(\frac{(n-m)\pi x}{a}\right)}{2(n-m)\pi/a} - \frac{\sin\left(\frac{(n+m)\pi x}{a}\right)}{2(n+m)\pi/a} \right]_{x=0}^{x=a} \\ &= A_n A_m \left[\frac{\sin((n-m)\pi)}{2(n-m)\pi/a} - \frac{\sin((n+m)\pi)}{2(n+m)\pi/a} - 0 + 0 \right] \end{aligned}$$

Since both n and m are integers, $n+m$ and $n-m$ will be integers as well and both sine terms will vanish. Hence, for any $n \neq m$, the integral will vanish. As such, any pair of functions in this set are mutually orthogonal, or the functions form an orthogonal set.

But what happens when $n = m$? Again, it is useful to pull the following result from a standard table of integrals.

$$\int \sin^2(\alpha x) dx = \frac{x}{2} - \frac{\sin(2\alpha x)}{4\alpha}$$

Substitution into this expression yields the following:

$$A_n^2 \int_{x=0}^{x=a} \sin^2\left(\frac{n\pi\, x}{a}\right) dx\, A_n^2 \left[\frac{x}{2} - \frac{\sin\left(\frac{2n\pi\, x}{a}\right)}{4\,(n\pi/a)}\right]_{x=0}^{x=a}$$

$$= A_n^2 \left[\frac{a}{2} - 0 - 0 + 0\right]$$

A convenient result comes from choosing values for A_n such that the result is unity.

$$1 = A_n^2 \left(\frac{a}{2}\right) \text{ or } A_n = \sqrt{\frac{2}{a}}$$

A_n is called a **normalization constant**, and has a value chosen to insure that the integral of the square of the function over all relevant space is unity. Another way of saying this is that A_n is chosen so as to **normalize** the function. We will see this concept throughout our development of quantum mechanics. Note that A_n does not depend on n. (This will not be the case for most normalization constants.)

These functions

$$X_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi\, x}{a}\right) \quad n = 1, 2, 3 \ldots$$

form an orthonormal set of functions. The have the property that

$$\int_{x=0}^{x=a} X_n X_m dx \ = \delta_{nm}$$

where δ_{nm} is the *Kronecker delta* and has the property

$$\delta_{nm} = \left| \begin{array}{l} 1 if n = m \\ 0 if n \neq m \end{array} \right.$$

The Time Solutions

The solution to the time dependence part of the problem is very similar to that of the spatial part. Recall that the equation

$$\frac{d^2}{dt^2} T(t) \ = \ -v^2 k^2 T(t)$$

must be satisfied. The value of k has already been determined from the special solutions and is given by $k = \frac{n\pi}{a}$. For convenience, let's make the substitution

$$\omega_n = vk = \frac{vn\pi}{a}$$

such that ω_n gives a frequency to the oscillation of the string that is parameterized by the velocity of the wave. Further, if n is doubled, the frequency of the wave is doubled. This would be manifested in the audible tone of the vibrating string going up by one octave. Those familiar with the acoustic nature of overtones on strings (such as those that can be produced on the strings of a guitar) are familiar with this concept.

The substitution creates the rather familiar looking eigenvalue-eigenfunction problem

$$\frac{d^2}{dt^2} T(t) \ = \ -\omega_n^2 T(t)$$

As was the case in the spatial part, the second order ordinary differential equation must have two linearly independent solutions, and any linear combination of those two functions will also be a solution to the equation. Thus, one can write

$$T(t) = C\sin(\omega_n t) + D\cos(\omega_n t)$$

The rest of the development requires a simple trick. Since there are no remaining boundary conditions by which we can evaluate C and D, we can choose a constant \sigma such that

$$C = -\sin(\delta) \text{ and } D = \cos(\delta)$$

so that the time function can be expressed

$$T(t) = \cos(\omega_n t)\cos(\delta) - \sin(\omega_n t)\sin(\delta)$$

and since

$$\cos(\alpha + \beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$$

the function can be expressed

$$T(t) = \cos(\omega_n t + \delta)$$

In this expression, σ is a phase shift in time. For a given choice of $t = 0$, σ can be forced to be zero. Given this constraint, the time function can be expressed

$$T(t) = \cos(\omega_n t)$$

The final result, then, for the normalized **wavefunctions** that describe the motion of the string are given by

$$\phi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi\, x}{a}\right)\cos(\omega_n t)$$

The Superposition Principle

For the following discussion, we will only concern ourselves with the time-independent solutions (the spatial functions) for simplicity. The time functions could be included to give the time evolution of each component of a superposition of waves, but the discussion of the mathematics involved would be identical to that for the spatial part of the problem. As such, we will focus just on the result for a fixed point in time of $t = 0$.

As it turns out, any well-constructed wave (specifically one that obey the boundary conditions of the original problem) can be expressed as a linear combination of normal mode waves.

$$\Phi(x) = \sum_n c_n \cdot X_n(x)$$

where \Phi(x) gives the function that describes the shape of the arbitrary wave, $X_n(x)$ are the time-independent functions that were derived in the previous section, given by

$$X_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi\, x}{a}\right)$$

And the factor c_n gives the amplitude of the n^{th} component of the superposition.

The coefficients c_n (known as **Fourier coefficients**) are easily calculated from the following expression

$$c_n = \int \Phi(x) \cdot X_n(x)\, dx$$

This is easily shown by making the substitution $\Phi(x) = \sum_m c_m X_m(x)$ into the above equation.

$$\begin{aligned} c_n &= \int \Phi(x) \cdot X_n(x)\, dx \\ &= \int \left(\sum_m c_m X_m(x)\right) X_n(x)\, dx \end{aligned}$$

Since integration is a linear operation, and multiplication is distributive, the result can be simplified

$$\begin{aligned} \int \left(\sum_m c_m X_m(x)\right) X_n(x)\, dx &= \sum_m c_m \int X_m(x) X_n(x)\, dx \\ &= \sum_m c_m \delta_{mn} \end{aligned}$$

using the orthonormality property of the functions $X_n(x)$ as developed above. The sum is also easy to simplify based on the properties of the Kronecker delta.

$$\begin{aligned}\sum_m c_m\delta_{mn} &= c_1\delta_{1n} + c_2\delta_{2n} + c_3\delta_{3n} + \ldots + c_n\delta_{nn} + \ldots \\ &= c_1\cdot 0 + c_2\cdot 0 + c_3\cdot 0 + \ldots + c_n\cdot 1 + \ldots \\ &= c_n\end{aligned}$$

The description of the function $\Phi(x) = \sum_n c_n X_n(x)$ is known as a Fourier expansion, and is the same sort of mathematics used by a Fourier Transform spectrometer. The spectrometer, through interferometry, measures the values of the amplitudes (c_n) and then mathematically reconstructs the spectrum by superimposing the constituent functions X_n(x) and adding them all up.

To illustrate the concept, consider a function that is defined as

$$\Phi(x) = \left| \begin{array}{lll} \sqrt{\frac{\pi}{2a}}\sin\left(\frac{2\pi x}{a}\right) & \text{if} & 0 \le x \le a/2 \\ 0 & \text{if} & a/2 \le x \le a \end{array}\right.$$

This function can be expanded in the **basis set** of normal mode (time independent) functions. The following MathCad worksheet calculates the values of the coefficients and demonstrates the superposition of waves.

This sort of expansion in a set of basis functions occurs throughout chemistry including the construction of an sp^3 hybridized orbital set used in the description of bonding in a methane molecule or the addition of p-orbitals to for π-bonding and antibonding orbitals. Expect to see this concept again!