Chemistry 331 **Assignment #3** (due Tuesday, October 13, in class)

It's impossible to overestimate the importance of **waves** in chemistry, physics, and other branches of science and technology! Sound waves we are familiar with move through gases, liquids and solids. Light and other radiation can be interpreted as ripples in the electric and magnetic fields. Electric circuits carry voltage and current waves. Quantum mechanical wave functions describe all of the measurable properties of atoms and molecules. *Etc.* The purpose of this assignment is to illustrate the basic properties of the **classical wave equation**.

1. Consider a string of length L fixed at both ends ($x = 0$ and $x = L$) and stretched horizontally. When the string is "plucked", like a guitar string, it begins to vibrate:

The vibration of the string obeys the one-dimensional **wave equation** from classical physics:

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \mathrm{v}^2 \frac{\partial^2 u(x,t)}{\partial x^2} \qquad (1)$$

$u(x,t)$ is the vertical displacement of the string from its initial horizontal position at position x and time t. The wave equation is a **partial differential equation**. What does "partial" mean in this context? [1]

2. The wave equation describes the vibration of the string, but to calculate the displacements of the vibrating string, the wave equation must be **solved** for $u(x,t)$. This can be done using the method of **separation of variables**. In this approach, the function $u(x,t)$ is assumed to be the product of the function $X(x)$ that depends only on position x and the function $T(t)$ that depends only on the time t.

$$u(x,t) = X(x)T(t) \qquad (2)$$

Substitute eqn (2) into eqn (1) and show the wave equation becomes [3]

$$\frac{1}{X(x)}\frac{\mathrm{d}^2 X(x)}{\mathrm{d}x^2} = \frac{1}{\mathrm{v}^2 T(t)}\frac{\mathrm{d}^2 T(t)}{\mathrm{d}t^2} \qquad (3)$$

3. The left side of eqn (3) is a function *only of* x, while the right side is function of *only of* t. x and t are independent variables. As a result, eqn (3) can hold for all values of x and t only if the left and right sides of the equation equal a constant, independent of x and t. Using $-\alpha^2$ for this constant gives

$$\frac{1}{X(x)}\frac{\mathrm{d}^2 X(x)}{\mathrm{d}x^2} = -\alpha^2 \qquad (4) \qquad\qquad \frac{1}{\mathrm{v}^2 T(t)}\frac{\mathrm{d}^2 T(t)}{\mathrm{d}t^2} = -\alpha^2 \qquad (5)$$

Notice that the wave equation, a partial differential equation, has been reduced to two separate ordinary differential equations. What is an **ordinary differential equation**? Why is an ordinary differential equation generally easier to solve than a partial differential equation? [2]

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4. A very simple rearrangement of eqn (4) for $X(x)$ gives

$$\frac{d^2X(x)}{dx^2} = -\alpha^2 X(x) \tag{6}$$

Notice that taking the second derivative of $X(x)$ gives $X(x)$ times the constant $-\alpha^2$. Use this information and the well known derivatives $d^2\sin(\alpha x)/dx^2 = -\alpha^2\sin(\alpha x)$ and $d^2\cos(\alpha x)/dx^2 = -\alpha^2\cos(\alpha x)$ to show that

$$X(x) = c_1\sin(\alpha x) + c_2\cos(\alpha x)$$

is a solution of eqn (6), with constants c_1 and c_2. [2]

5. The vibrating string is fixed at both ends, so $X(0) = 0$ and $X(L) = 0$ at all times. As a consequence of these **boundary conditions**, prove c_2 is zero and show that $X(x)$ is the sine function

$$X(x) = c_1 \sin\left(\frac{n\pi x}{L}\right) \qquad n = 1, 2, 3, \ldots$$

with $\alpha = n\pi/L$ for **integer values of *n***. *This result is important!* Because electrons behave like waves, quantum mechanical wave equations have solutions only for integral values of certain variables. This is the origin of **quantum numbers** and **discrete energy levels**. [2]

6. Show $X(x)$ is the equation for a **standing wave** (*i.e.*, "stationary" wave) with wavelength $\lambda = 2L/n$. [1]

7. By defining $\omega = \alpha v$, show that a simple rearrangement of eqn (5) gives

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

which has the solution

$$T(t) = c_3\sin(\omega t) + c_4\cos(\omega t) \tag{7}$$

with constants c_3 and c_4. [2]

8. The time function $T(t)$ describing the wave oscillates with **angular frequency ω**. In other words, there is one complete oscillation, from angle $\omega t = 0$ to angle $\omega t = 2\pi$ radians, every $2\pi/\omega$ seconds. Show that the **frequency ν** of the oscillation (the number of oscillations per second) is therefore

$$\nu = \omega/2\pi$$

so one wave of length λ goes by every ν^{-1} seconds. To complete this introduction to the wave equation, show that v in the wave equation [eqn (1)] is the **speed of the moving wave**, $\mathrm{v} = \lambda\nu$. [1]

It can be shown that $\mathrm{v} = (T/\rho)^{1/2}$, where T is the tension in the string and ρ is the mass of the string per unit length, so high velocity waves are predicted for light strings under high tension.

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Q1. The displacement of the string, $u(x,t)$, is a function of **two** independent variables: position x and time t.

This means that $\dfrac{\partial^2 u(x,t)}{\partial t^2} = \left(\dfrac{\partial^2 u}{\partial t^2}\right)_x$ is a partial derivative.
(x is held constant while taking the "partial" t derivative.)

Similarly, $\dfrac{\partial^2 u(x,t)}{\partial x^2} = \left(\dfrac{\partial^2 u}{\partial x^2}\right)_t$ is a "partial" x derivative. (t is held constant.)

Consequently, $\dfrac{\partial^2 u}{\partial t^2} = v^2 \dfrac{\partial^2 u}{\partial x^2}$ is a partial differential equation.

Q2. Substitute $u(x,t) = X(x)\,T(t)$ into wave equation (1):

$$\left(\frac{\partial^2 [X(x)\,T(t)]}{\partial t^2}\right)_x = v^2 \left(\frac{\partial^2 [X(x)\,T(t)]}{\partial x^2}\right)_t$$

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

"ordinary" derivatives of functions of one variable

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

Q3. $\dfrac{1}{v^2 T(t)}\,\dfrac{d^2 T(t)}{dt^2} = -\alpha^2$ and $\dfrac{1}{X(x)}\,\dfrac{d^2 X(x)}{dx^2} = -\alpha^2$

are ordinary differential equations containing derivatives of functions of a single variable (x or t)

use: $\boxed{\frac{d^2}{dx^2}[c_1 \sin(\alpha x)] = c_1 \frac{d}{dx}\frac{d}{dx}\sin(\alpha x) = c_1 \frac{d}{dx}[\alpha\cos(\alpha x)] = c_1(\alpha)(-\alpha)\sin(\alpha x) = -\alpha^2 c_1 \sin(\alpha x)}$

Q4. Substitute $X(x) = c_1 \sin(\alpha x) + c_2 \cos(\alpha x)$ into $\frac{d^2 X(x)}{dx^2} = -\alpha^2 X(x)$

$$\frac{d^2}{dx^2}[c_1 \sin(\alpha x) + c_2 \cos(\alpha x)] = c_1 \frac{d^2 \sin(\alpha x)}{dx^2} + c_2 \frac{d^2 \cos(\alpha x)}{dx^2}$$

$$= -c_1 \alpha^2 \sin(\alpha x) - c_2 \alpha^2 \cos(\alpha x)$$

$$= -\alpha^2 [c_1 \sin(\alpha x) + c_2 \cos(\alpha x)]$$

$$= -\alpha^2 X(x)$$

Similarly:

$$\frac{d}{dx}\frac{d}{dx}\cos(\alpha x) = \frac{d}{dx}[(-\alpha)\sin(\alpha x)] = -\alpha^2 \cos(\alpha x)$$

Q5. $X(0) = 0 = c_1 \sin(0) + c_2 \cos(0) = c_1(0) + c_2(1)$

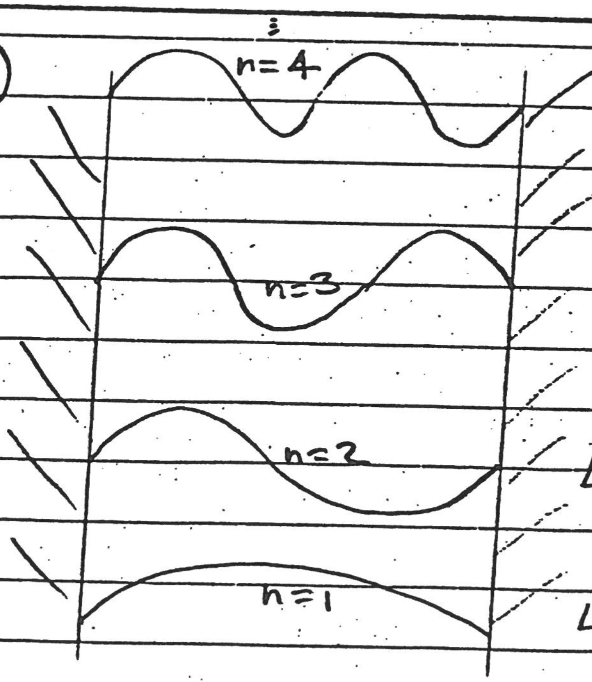
$0 = c_2 \quad \therefore \; X(x) = c_1 \sin(\alpha x)$

$X(L) = 0 = c_1 \sin(\alpha L)$ recall: $\sin(\pi) = \sin(2\pi) = \sin(3\pi) = \dots = 0$

$\therefore \; \alpha L = \pi, 2\pi, 3\pi, \dots$ or $\alpha = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \dots$

and $X(x) = c_1 \sin\left(\frac{n\pi x}{L}\right)$

Q6.



$L = 2\lambda = \frac{4\lambda}{2}$

$L = \frac{3}{2}\lambda$

$L = \lambda = \frac{2\lambda}{2}$

$L = \frac{\lambda}{2}$

$L = \frac{n\lambda}{2}$

$n = 1, 2, 3, \dots$

$\lambda = \frac{2L}{n}$

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Q7. Substitute $T(t) = c_3 \sin(\omega t) + c_4 \cos(\omega t)$

into $\dfrac{d^2 T(t)}{dt^2} = -\omega^2 T(t)$

$$\frac{d^2}{dt^2}\left[c_3 \sin(\omega t) + c_4 \cos(\omega t)\right] = c_3 \frac{d^2 \sin(\omega t)}{dt^2} + c_4 \frac{d^2 \cos(\omega t)}{dt^2}$$

$$= -c_3 \omega^2 \sin(\omega t) - c_4 \omega^2 \cos(\omega t)$$

$$= -\omega^2 \left[c_3 \sin(\omega t) + c_4 \cos(\omega t)\right]$$

$$= -\omega^2 T(t)$$

Q8. $\dfrac{d^2 T(t)}{dt^2} = -\omega^2 T(t) = -\alpha^2 v^2 T(t)$ (from Q2)

$$\omega^2 = \alpha^2 v^2$$

$$\omega = \alpha v$$

combine $\alpha = \dfrac{n\pi}{L}$ (Q5) and $L = \dfrac{n\lambda}{2}$ (Q6)

$$\omega = \alpha v = \frac{n\pi}{L} v = \frac{n\pi}{\frac{n\lambda}{2}} v = \frac{2\pi v}{\lambda}$$

$$v = \frac{\omega}{2\pi}\lambda = \nu\lambda$$ (wave velocity v in terms of the frequency ν and the wavelength)