**Supplement 1: Chemistry 6854**

**Physical Chemistry Alfred State College**

 **Derivation of the classical 1-D wave equation (eq. 2.1 p. 40 of text)**

McQuarrie starts chapter 2 page 39 by asserting that the solution to the 1-dimensional `wave’ equation, (see **1** below) is a good model for Schrodinger’s quantum mechanical description of matter. Thus, if we can work our way through the analysis of this classical problem, we are well-positioned to tackle the central problem in quantum mechanics: Schrodinger’s equation.

**1 \_1\_ \* ∂2u (x,t) = ∂2u(x,t) classical 1 D wave equation**

**υ2 ∂t2  ∂x2**

 While it is quite possible to work through the mathematical solution of this equation with no understanding of how it came about or what it is trying to explain, it is obviously helpful and better if we understand the origins of the equation. Understanding physics lies not in knowing the equations but in the intervening reasoning that leads to the equations.

**Force picture**

If we imagine a string tied tightly between two walls, then the basic physical situation is that there is no net Force along x, but only along u(x,t) since the string stays in one place.

 **Figure 1: Tension picture**

 **u=y**

Thus, any applied Force occurs along the y axis = u axis wall

 T(x) T(x+Δx)

**2** F=ma = m d2u(x,t)

 dt2 **x🡪**

 x x+Δx

where `m’ is a section of the string mass between x and x +Δx. The value of the force can be computed given the tension initially impressed by plucking the string.

The tension, T is a constant and can be thought of as the `force’ applied to every point of the string and in the direction of the string. Note that the string cannot change dimension, e.g. L= fixed, and the tension, T is produced by pulling the string upwards at some point along the x axis. We expect as noted above, that the sustainable motion of that string after release will be sinusoidal, and we assume the string does not undergo some sort of heating or hysteresis as it vibrates. The T produces the vertical displacement of u(x,t) , which will vary as function of x and t

To find the value of that force on the string mass m between x and x + Δx in terms of T we use some geometry and an approximation as Δx gets small.

Derivation of the classical, 1-D wave equation (continued)

At x, the downward force Fx ~ T sin θ

But we assume the u(x,t) is small versus L

so the angle θ is small. At small angles:

sin θ🡪 tan θ🡪 du/dx.

So: F­x =downward force = Tdu(x,t)

 dx

A similar conclusion applies to x+Δx, except that it is taken as a the net upward force Fx+Δx = upwards force =Tdu(x+Δx,t)

 **Figure 2: geometry of vertical forces vs T**

 θ

 δx

 x x +Δx

 dx

**3** Thus: F= m∂2u (x,t) = Fx+Δx -F­x = T[(du(x+Δx,t) - du(x,t)]

 ∂t2 dx dx

We can re-express u(x+Δx,t) ~ u(x,t) + du(x,t)\* Δx and substitute into  **3**

 dx

**4** Thus: F= m∂2u (x,t) = T[(du +d2u Δx - du] = Td2u \*Δx

 ∂t2 dx dx2 dx dx2

Since m = mass of string segment = ρΔx where ρ = string density in c.a. g/cm:

**5a** ρ ∂2u (x,t) = ∂2u

T ∂t2  ∂x2

Note that T is in units of g cm/sec2 so:

 ρ/T= g/cm \* 1/(g cm sec-2) = (s/cm)-2 = 1/(velocity)2 =1/υ2

 υ= velocity of displacement wave across x

**5b \_1\_ ∂2u (x,t) = ∂2u**

 **υ2 ∂t2  ∂x2**