Phys 304: Assignment 3

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This problem set took me an absurd amount of time because of the approximation method I chose for the first question. I estimate that it took me about 20 hours to do this problem set. I did, however, learn a lot about recursive functions, functions within functions, and when to call those functions. My collaborators for this problem set were Luke Smithberg and Melanie Santiago.

1. PROBLEM 1: THE TRIG LIBRARY

In order to approximate the trigonometric functions, my collaborators and I chose to use Bhaskara's Sine Approximation. Bhaskara was a 7th century Indian mathematician who created an incredibly accurate approximation for the sine function[1]. His derivation of the approximation was not well documented, although the approximation itself has survived. Stroethoff[1] goes through a possible derivation for this. Bhaskara's approximation formula is as follows:

$$\sin\theta^\circ \approx \frac{4\theta(180-\theta)}{40500-\theta(180-\theta}. \tag{1}$$

Using this, approximations of the sine, cosine, and tangent functions can be graphed with their error.

1.1. The sine function

The pseudocode to create a plot of the sine function is shown in Figure 1. The input angle $x < 180$ is halved until machine precision dictates the Bhaskara function of the next half is equivalent to the Bhaskara function of the previous value. Then using the double angle formula,

$$\sin 2x = 2\sin 2\sqrt{1-\sin x^2}, \tag{2}$$

previous angles are recursively added to generate the Bhaskara function of the original angle. This is necessary to obtain the smallest error possible in the calculation of the sine.

Using the method in Figure 1, a graph of the approximation of the sine function can be generated.

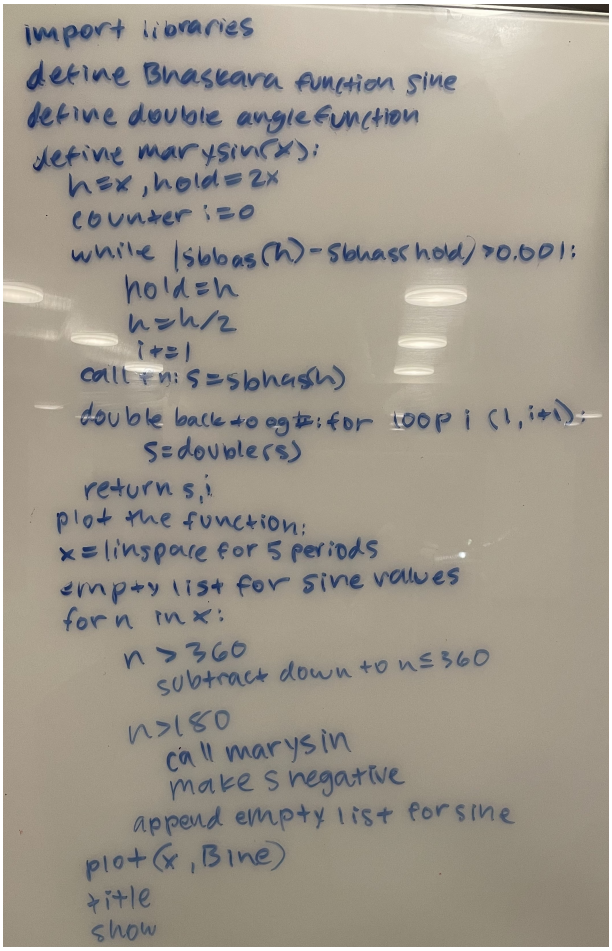

FIG. 1: [The psuedocode for the creation of the sine plot.]

1.2. The cosine function

Using the identity

$$\cos x = \sqrt{1-\sin x^2}, \tag{3}$$

cosine values can be created from the sine values. The pseudocode to create a plot of the cosine function can be found in Figure 3.

From this method in Figure 3, code to graph the approximation of the cosine function can be generated.

1.3. The tangent function

Using the identity

$$\tan x = \frac{\sin x}{\cos x} \tag{4}$$

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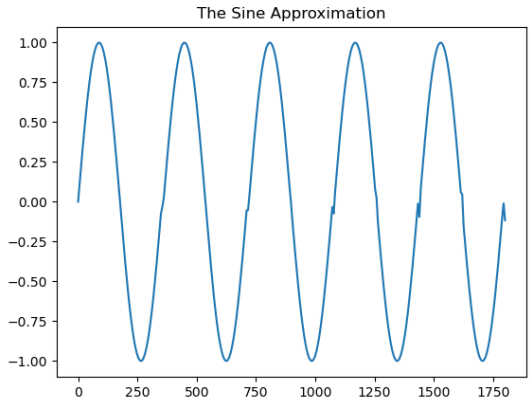

FIG. 2: [Approximation of the sine function using Bhaskara's function.]

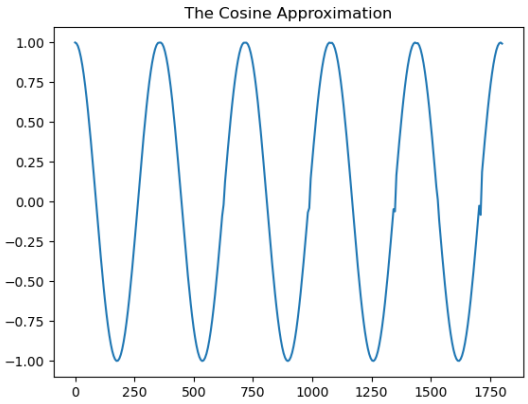

FIG. 4: [Approximation of the cosine function using Bhaskara's function.]

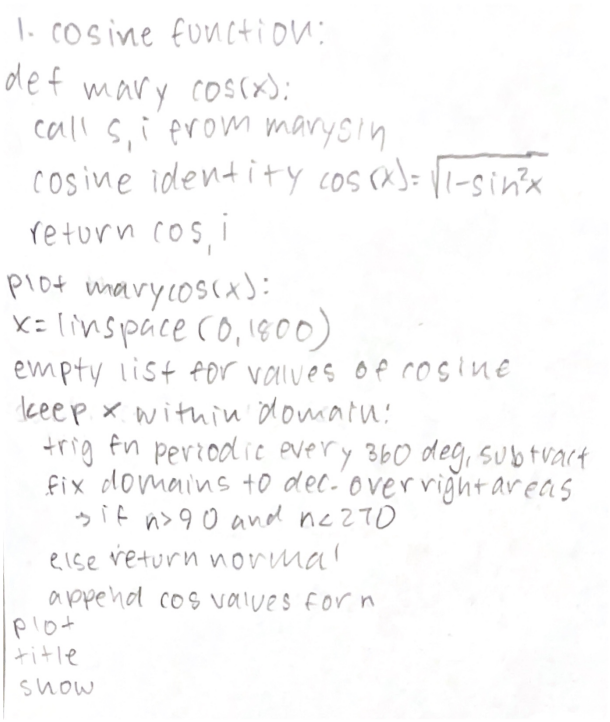

FIG. 3: [The psuedocode for the creation of the cosine plot.]

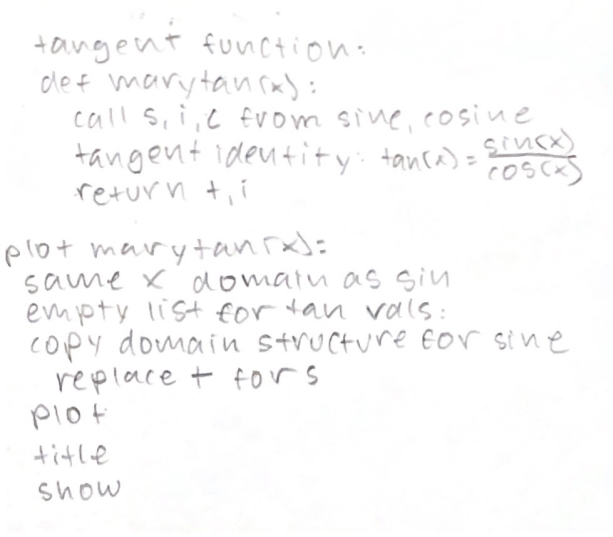

FIG. 5: [The psuedocode for the creation of the tangent plot.]

tangent values can be generated from the original sine values and the cosine values found in Section 1.2. The pseudocode to create a plot of the tangent function can be found in Figure 5.

Using this method in Figure 5, a graph of the approximation of the tangent function can be generated.

What is interesting to note from Figure 8 is how the computer processes the asymptotic behavior of the tangent function. The asymptote at 270° reaches a value of almost -300. This is due to the fact that this function is based off an approximation for sine and cosine. So, the cosine values aren't actually reaching precisely zero where it should be. This means the tangent function is dividing a number by a very tiny number, which yields values reaching almost -300.

1.4. The error function

The error function

$$\epsilon = \frac{|calc - obs|}{obs} \tag{5}$$

can be used to generate the error between observed and calculated values to find the error in calculated values. This method can be applied to this approximation by taking the angle past the most accurate halved angle of the Bhaskara function as the calculated value, and taking

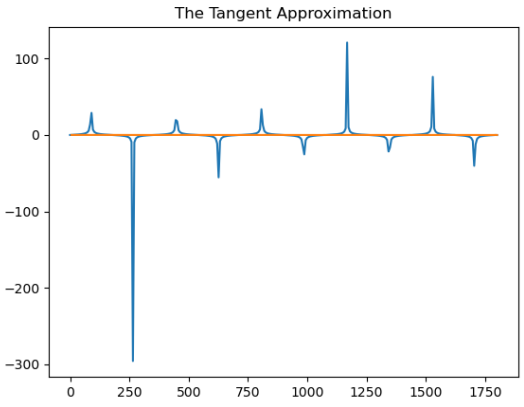

FIG. 6: [Approximation of the tangent function using Bhaskara's function.]

the most accurate halved angle as the observed value. This method is described in Figure 7.

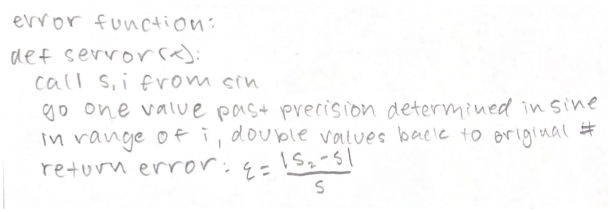

FIG. 7: [The pseudocode for the creation of the error plot.]

A plot of the error approximation can then be generated.

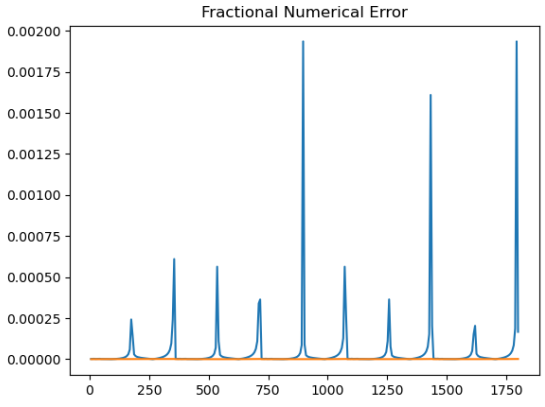

FIG. 8: [The plot of the error function from using Bhaskara's function.]

2. PROBLEM 2: THE MADELUNG CONSTANT

The Madelung constant is a quantity related to the geometric structure of materials[2]. Ionic solids are made up of a lattice structure of charged particles each with their own electrostatic potential. The charged particles, or ions, each have alternating charges in order to maintain their shape. This creates an interesting effect, as oppositely charged ions in the structure will attract and the same charges will repel. So, it is useful to know information about the Madelung constant for a solid. The constant is then used to derive the Madelung energy, which yields the lattice energy of the structure. The lattice energy determines many physical properties of the material.

2.1. Plotting the constant

The Madelung constant is given by:

$$M = \sum_{j,k,l=-\infty}^{\infty} \frac{(-1)^{j+k+l}}{\sqrt{j^2+k^2+l^2}} \tag{6}$$

Using the process described in Figure 9, code to generate a plot of the Madelung constant can be created.

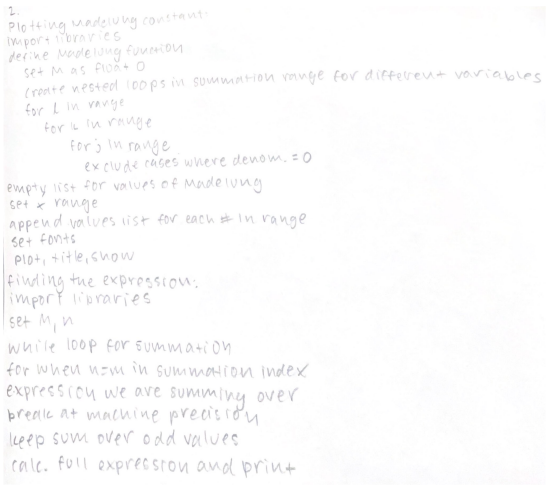

FIG. 9: [The pseudocode for the creation of the Madelung plot and expression comparison.]

The plot of the Madelung constant is given in Figure 10.

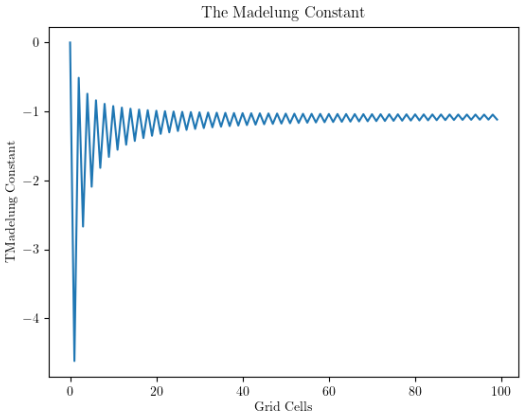

FIG. 10: [The plot of the Madelung function, described in Equation 6.]

The expression

$$M = 12\pi \sum_{m,n\geq 1,odd} sech^2(\frac{\pi}{2}\sqrt{m^2+n^2}) \qquad (7)$$

gives a possible solution for the Madelung constant. Using the process described in Figure 9, this yields a result $M \approx 1.7475$, which lies on the curve in Figure 10.

[1] K. Stroethoff, The Mathematics Enthusiast (2014).
[2] L. Glasser, Inorganic Chemistry (2012).