PHYS 304 AS3

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1. TRIG LIBRARY

In this problem, we define our trig functions. As the first step, we define a function by giving it a name. Given the input value, we normalize the x input from 0 to 2π. Then, we initialize an iterator i by setting $i = 0$. Then, we initialize two variables s and *sold* by setting them to 0. Then, we start a loop where we utilize the Taylor series. We include a line "sold=s," which helps to check the convergence later. Then, we have the summation function for the Taylor series. For sin, we have $\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n}$. In the code, we use $s+=$ to represent the summation part. After this, we give a statement "if sold==s: break" combined with the line "sold=s," which can be used to check convergence. Figure 1 shows 5 periods of our trig functions. The legend indicates the specific function.

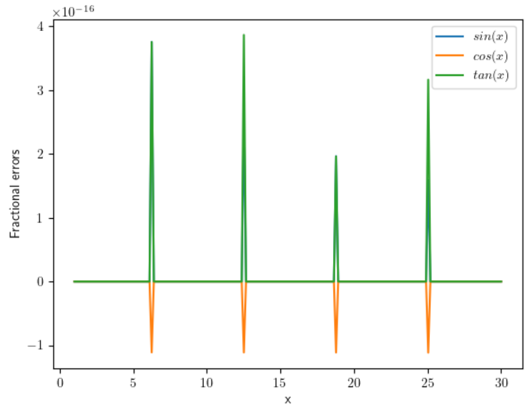

FIG. 2: [Fractional error of our trig functions.]

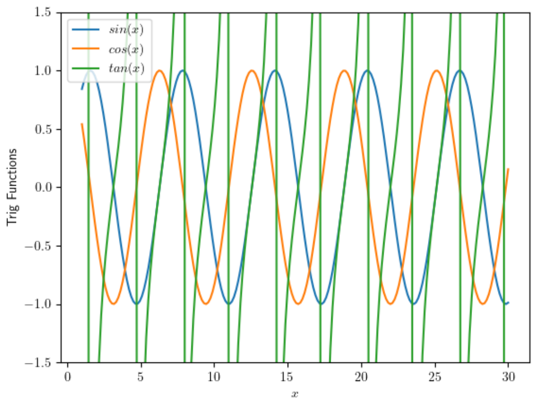

FIG. 1: [Our Trig function.]

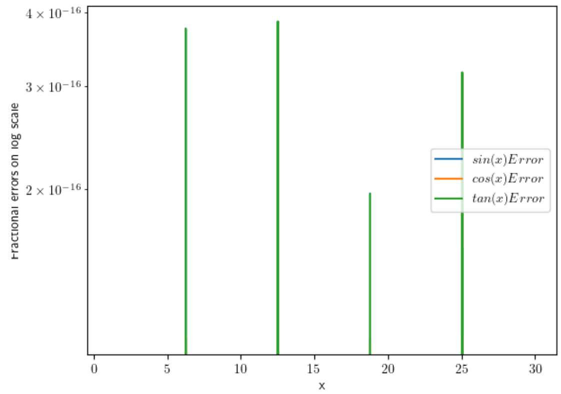

FIG. 3: [Fractional error of our trig functions on log scale.]

Figure 2 shows the fractional errors. The way we calculate the error is: for the loop inside the trig function, I used 20 in my trig library. To have a more accurate calculation, I define another set of trig functions with 10000 loops. Then, I subtract the two sets and divide by the more accurate library to get the fractional error. As we can tell from figure 2, the values are on the order of 10^{-16}, which indicates my trig library is a very good estimate. Then, in figure 3, the axis was set on the log scale for a clearer view.

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2. MADELUNG CONSTANT

For this problem, we are given two equations. The first one is $M = \sum_{j,k,l=-\infty}^{\infty} \frac{(-1)^{j+k+l}}{\sqrt{j^2+k^2+l^2}}$. Firstly, I define a function; inside the function, give a parameter and set it to 0. This will be the final output after rounds of add-ons. Since we have three iterations j, k, and l, we will have three loops. The order I defined is l loop inside the loop k, then k loop inside the j loop. Notice the denominator: we want to avoid the case when $j = k = l = 0$, which will blow the computer's brain. Inside the last loop, we set a statement that "if j==k==l==0: continue," so the loop will skip this case. Then we enter our function. Similar to the trig function problem, we use + = to represent the summation. Figure 4 shows the Madelung constant plot. The plot shows a decaying sinusoidal behavior, which stabilizes at 1.75. The x-axis represents the area that we focus on the lattice. The bigger the N is, the more lattice our calculation covers.

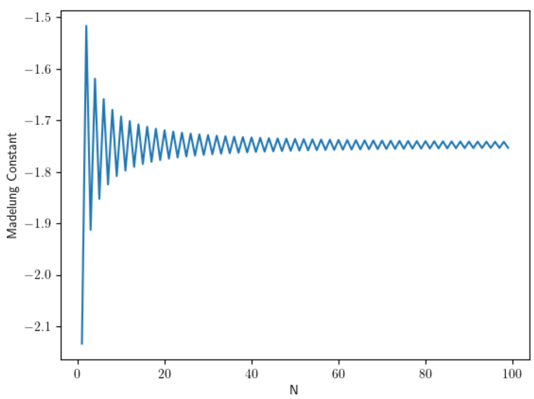

FIG. 4: [Madelung Constant with Equation 1]

In a very similar way, we define the second equation and make a plot. Figure 5 shows the behavior defined by this function, which doesn't have any oscillation as figure 4.

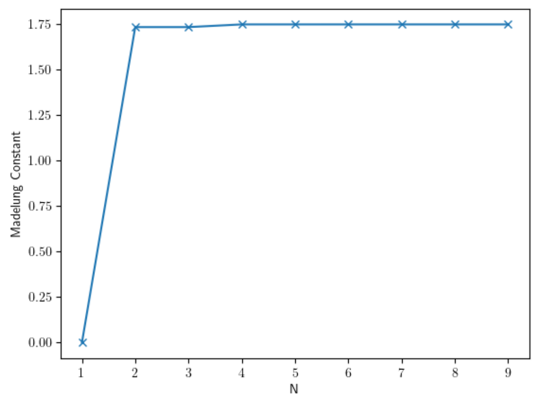

FIG. 5: [Madelung Constant with Equation 2]

For the third part, I explore another way to calculate the Madelung constant. The equation I explore is,

$$M = \frac{\pi}{2} + 3 \sum_{u,v \in Z^2} \frac{(-1)^2 cosech(\pi r)}{r} \quad (1)$$

, where $r = (u^2 + v^2)^{1/2}$[1]. In this equation, we take into account the positive and negative charges. The $(-1)^v$ is where we alternate the change of charges. Here, we only have two variables, v and u. Both v and u are the length of a 3-vector, indicated by Z^3. This indicates that we have 6 dimensions. If we have a $Na - Cl$ crystal, we can use v and u to represent the Na^+ and Cl^- atom. The $(-1)^v$ represents the opposite charges on Na and Cl atoms. Figure 6 shows the plot of the Madelung constant defined by equation 1. It also converges to 1.75. However, there's a little bump reaching 1.76 when the constant tries to stabilize. My interpretation is that since we consider the change of charge signs, the little bump somehow represents the positive and negative charge interactions at some point. This means the attractive potential is bigger than the repulsive potential between like charges.

Madelung constant is essential for calculating the electric potential energy between atoms inside a crystal. It's important to understand the electric properties of materials. The constant can be modified in many ways to represent diverse electron distributions. For example, we can take into account the change of signs of charges, as we have shown in figure 6, which shows a similar converging value but a different behavior. With the Madelung constant, we can examine the interior potential energy of crystals and compare different crystals.

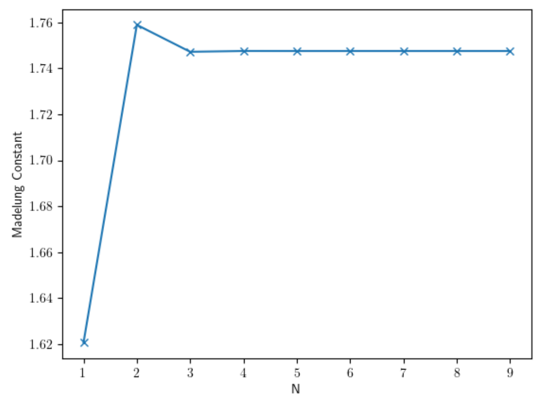

FIG. 6: [Madelung Constant defined by equation 1]

[1] R. E. Crandall and J. P. Buhler, Journal of Physics A: Mathematical and General **20**, 5497 (1987), URL https://dx.doi.org/10.1088/0305-4470/20/16/024.