Homework 3 Write-Up

Petra Budavari*
Haverford College Department of Physics
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1. TRIG LIBRARY

For this exercise, we created a group of functions for sine, cosine, and tangent in Python. I used Taylor series to define the trigonometric functions sine and cosine and used the resulting two functions to calculate tangent 3. Figure(1) shows my thought process. The function was set to break the Taylor series once the program could no longer tell the difference between the last Taylor series and the following one. To plot the functions to the input values of x, I had to use np.vectorize numpy function. Figure(2) gives the resulting plot.

$$Sin(x) \approx \sum_{n=0}^{1000} \frac{-1^n}{(2n+1)!} x^{2n+1} \quad (1)$$

$$Cos(x) \approx \sum_{n=0}^{1000} \frac{-1^n}{(2n)!} x^{2n} \quad (2)$$

$$Tan(x) = Sin(x)/Cos(x) \quad (3)$$

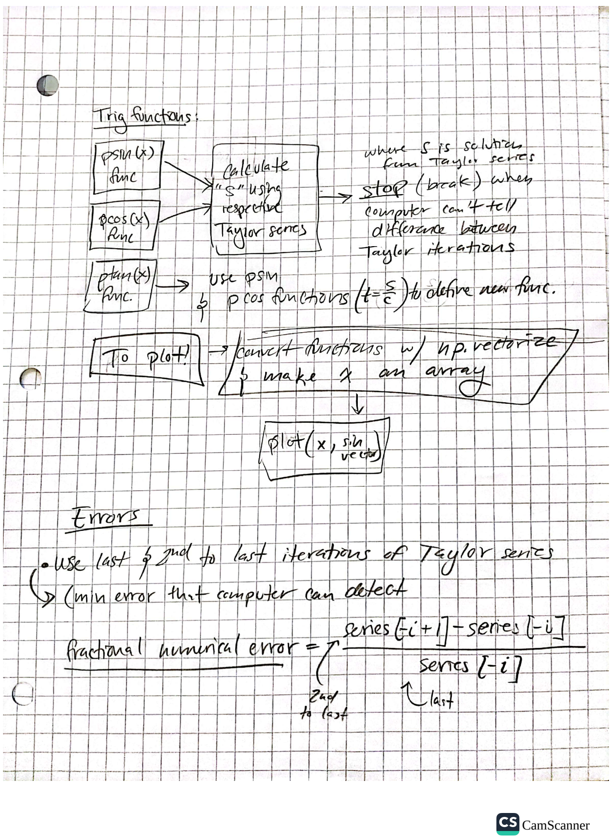

FIG. 1: Flow chart for Trig Library.

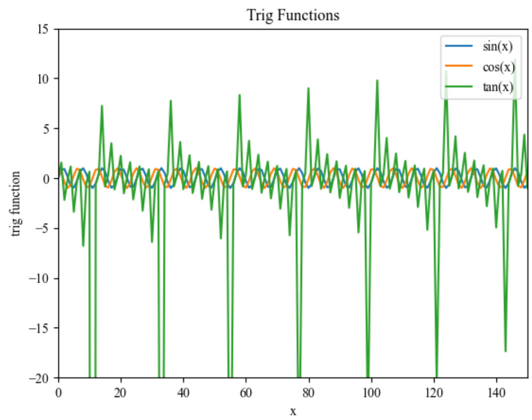

FIG. 2: Plot of "homemade" trig functions over values of x.

We were then asked to calculated the fractional numerical error of the functions we created. To do this, I calculated the fractional error using the last and second to last Taylor series when the difference between the two is under some small value 4. This does introduce the problem that now the fractional error is above some fixed value - there is likely a better way to do this.

$$Error = (\text{PreviousSeries} - \text{LastSeries})/\text{LastSeries} \quad (4)$$

I then plotted the fractional errors for all of the functions in my trig library Figure(3). The error are very small (on the order of e^-11) and you can see that the error of tangent(x) is affected by cos and sin errors.

2. MADELUNG CONSTANT

In this exercise, we plotted the Madelung constant. From Equ(5) you can see that the sum is taken from

*Electronic address: pbudavari@haverford

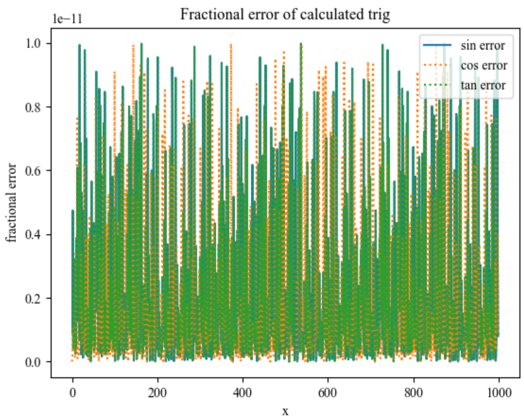

FIG. 3: Fractional error of trig functions.

negative infinity to positive infinity, however, the program cannot actually calculate this. Therefore, the lattice pattern was defined by a limited grid size. To use the sum of all three indices j,k,l, I created a system of nested for loops. Equ(5 lead to the plot seen in Figure(5) where you can see that the Madelung constant converges to the value -1.75.

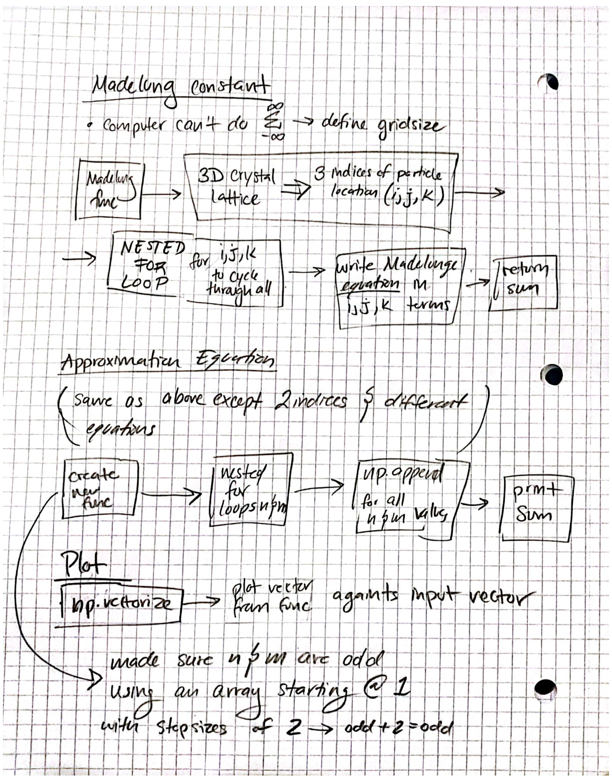

FIG. 4: Flow chart for calculating Madelung constant.

$$\text{Madelung Constant} = \sum_{j,k,l=-\infty}^{\infty} \frac{((-1)^{j+k+l}}{\sqrt{j^2+k^2+l^2}} \tag{5}$$

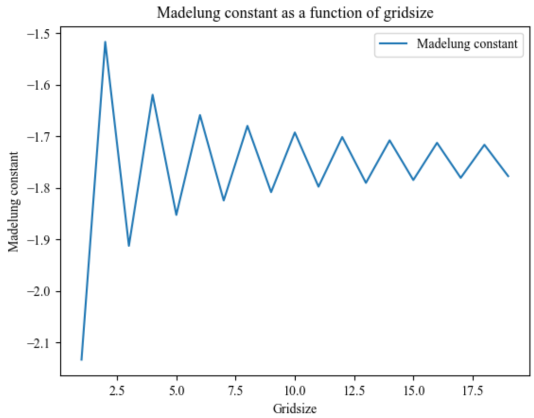

FIG. 5: Calculate Madelung constant.

I then plotted another equation of a very good approximation of the Madelung constant 6. This only took one nested for loop as there are only two variables. This result converges to approximately 1.75 (Fig.(6). I suspect that there is a change in sign because of the new assumption that all of the particle around the center particle are positively charges rather than negatively. Otherwise, the plots converge to the same Madelung constant.

$$\text{Madelung Approx.} = 12\pi \sum_{n,m\geq 1,odd} sech^2\left(\frac{\pi}{2}\sqrt{m^2+n^2}\right) \tag{6}$$

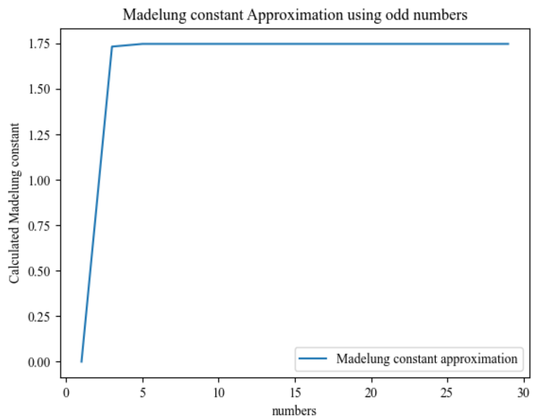

FIG. 6: Approximation for Madelung constant.

Lastly, I re-plotted the original Madelung equation but with changes to the lattice parameters. Now, the distance between particles along the j axis is ten times the original distance, twice the length for particles along the k axis and also t,he particles along the j vector have the same charge as the point we are measuring the Madelung constant from 7. This new Madelung constant converges to -1.4 as seen in Figure(7).

$$\text{My Madelung Constant} = \sum_{j,k,l=-\infty}^{\infty} \frac{((-1)^{-j+k+l}}{\sqrt{10j^2 + 2k^2 + l^2}} \tag{7}$$

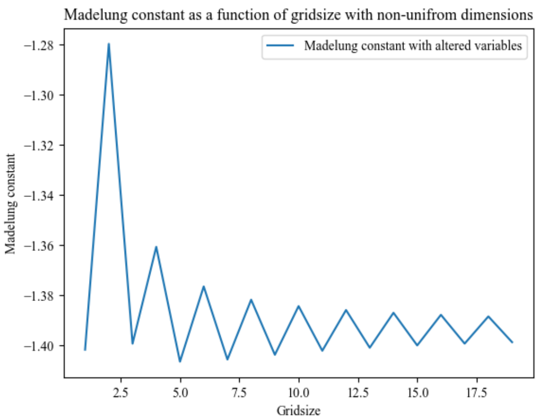

FIG. 7: Madelung constant with varied parameters.

The Madelung constant can be used the measure the electrostatic potential of any ion in a crystal lattice by approximated the charge density as a point charge [1]. This has very important application for understanding and characterizing crystal structures. It takes into account the attraction and repulsion forces between the ions and there have been many approximations for this calculation [2].

3. SURVEY QUESTIONS

The homework this week took approximately 8 hours (I was stuck on a bug for about 1.5 hours of that). I learned how to use nested for loops, how to build functions and vectorize them, and more general problem solving techniques. This homework was reasonable and useful.

[1] *Madelung constant*, URL https://en.wikipedia.org/wiki/Madelung_constant.

[2] *Libre texts, 5.11: Lattice energy - madelung constants*, URL https://chem.libretexts.org/Courses/Northern_Michigan_University/CH_215%3A_Chemistry_of_the_Elements_Fall_2023/05%3A_Solids_and_Solid-State_Chemistry/5.11%3A_Lattice_Energy_-_Madelung_Constants#:~:text=The%20Madelung%20constant%20takes%20in,from%20the%20distance%20between%20ions.