46.5+45+5 = 96.5

96.5/117

PHYS 304 AS3

Xiyue Shen*
Haverford College Department of Physics

(Dated: February 23, 2024)

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.

equations for cos and tan?

?

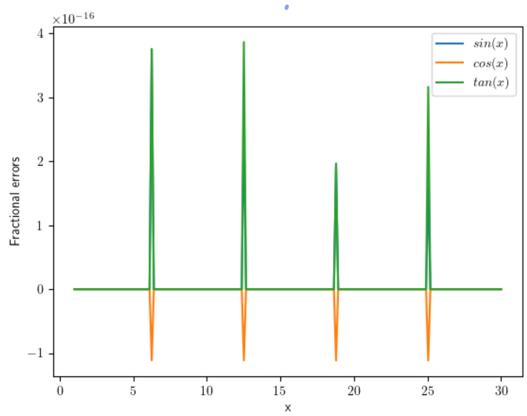

FIG. 2: [Fractional error of our trig functions.]

title?

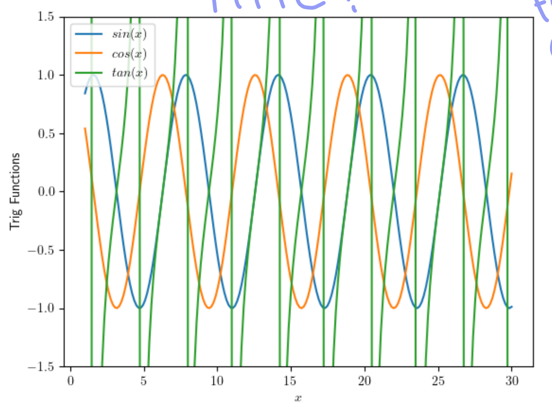

FIG. 1: [Our Trig function.]

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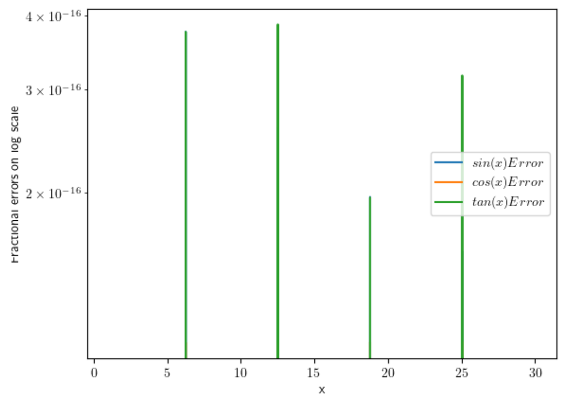

FIG. 3: [Fractional error of our trig functions on log scale.]

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.

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

*Electronic address: xshen2@brynmawr.edu; URL: Optionalhomepage

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.

explain why we are allowed to take abs value to compare results

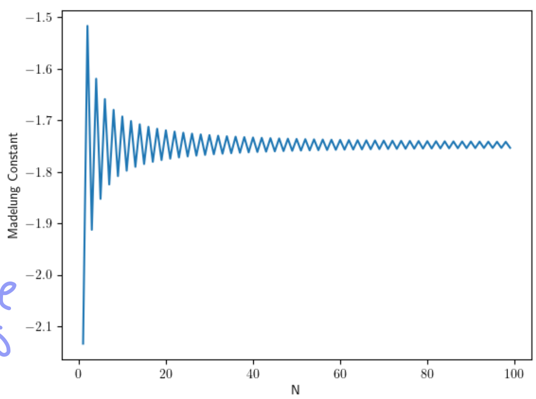

FIG. 4: [Madelung Constant with Equation 1]

typeset?

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.

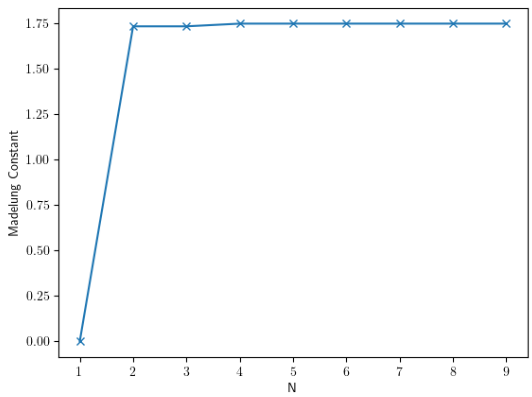

FIG. 5: [Madelung Constant with Equation 2]

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.

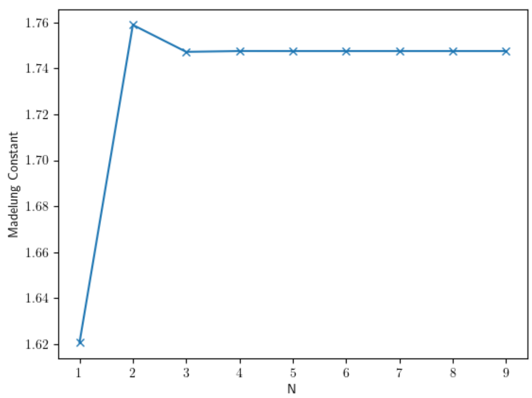

FIG. 6: [Madelung Constant defined by equation 1]

3. SURVEY

5

I took 6 hours to finish this week's homework. I learned how to make a plot in log scale, define a function, put a loop inside a loop, and initialize iteration. I like the Madelung problem most. I think the problem set is about the right length.

4. UNGRADED

I have downloaded the repository.
I have followed along with class notes and made sure everything makes sense.

psuedocode?

I have completed the tutorial to have a better understanding.

[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.

Q 1 46.5/56

Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics [1]

Haverford College, Prof. Daniel Grin

For coding assignments, roughly 56 points will be available per problem. Partial credit available on all non-1 items.

4 1. Does the program complete without crashing in a reasonable time frame? (+4 points)

2 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points)

3 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points)

5 4. Is the algorithm appropriate for the problem? If a specific algorithm was requested in the prompt, was it used? (+5 points)

4 5. If relevant, were proper parameters/choices made for a numerically converged answer? (+4 points)

4 6. Is the output answer correct? (+4 points).

3 7. Is the code readable? (+3 points)

. 5.1. Are variables named reasonably?

. 5.2. Are the user-functions and imports used?

[1] Inspired by rubric of D. Narayanan, U. Florida, and C. Cooksey, U. Hawaii

. 5.3. Are units explained (if necessary)?

. 5.4. Are algorithms found on the internet/book/etc. properly attributed?

1.5 8. Is the code well documented? (+3 points)

. 6.1. Is the code author named? please comment your name at the top of your code -1

. 6.2. Are the functions described and ambiguous variables defined?

good documentation on your first few equations, should keep this throughout -0.5

. 6.3. Is the code functionality (i.e. can I run it easily enough?) documented?

9. Write-up (up to 28 points)

0 . Is the problem-solving approach clearly indicated through a flow-chart, pseudo-code, or other appropriate schematic? (+5 points) please include psuedo-code -5

✓ . Is a clear, legible LaTeX type-set write up handed in?

3 . Are key figures and numbers from the problem given? (+ 3 points)

3 . Do figures and or tables have captions/legends/units clearly indicated. (+ 4 points) Figs need titles -1

3 . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points)

2 . Is a brief explanation of physical context given? (+2 points)

1 . If relevant, are helpful analytic scalings or known solutions given? (+1 point)

3 . Is the algorithm used explicitly stated and justified? (+3 points)

2 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

0 . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)

More typeset equations needed -2 [cos, tan, error]

1 . Are collaborators clearly acknowledged? (+1 point)

2 . Are any outside references appropriately cited? (+2 point)

Q. 2 45/56

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For coding assignments, roughly 56 points will be available per problem. Partial credit available on all non-1 items.

3 1. Does the program complete without crashing in a reasonable time frame? (+4 points)

code takes a long time to run -1

2 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points)

3 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points)

5 4. Is the algorithm appropriate for the problem? If a specific algorithm was requested in the prompt, was it used? (+5 points)

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4 6. Is the output answer correct? (+4 points).

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✓ . Is a clear, legible LaTeX type-set write up handed in?

3 . Are key figures and numbers from the problem given? (+ 3 points)

4 . Do figures and or tables have captions/legends/units clearly indicated. (+ 4 points)

3 . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points)

0 . Is a brief explanation of physical context given? (+2 points) explicitly compare the results from eq. 1 and 2 -2

1 . If relevant, are helpful analytic scalings or known solutions given? (+1 point)

3 . Is the algorithm used explicitly stated and justified? (+3 points)

1 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

need to explain why we can compare the magnitudes of the results -1

1 . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)

Need to include all equations from problem

1 . Are collaborators clearly acknowledged? (+1 point)

−1

2 . Are any outside references appropriately cited? (+2 point)