PHYS 304 AS5

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No Collaborators. I have two python files.

PHYS_304_HW5_5.13_Xiyue_Shen.py file is the Quantum harmonic oscillator problem, numbered as 5.13 in the textbook.

PHYS_304_HW5_Simpson code up_Xiyue_Shen.py is the file for in-class free-choice integration exercise

1. SIMPSON'S METHOD

1.1. Equation Setup

In this problem, I aim to use Simpson's method to examine the integral. Simpson's method chooses three points and finds the equation of a quadratic through those points. The basic idea is that suppose we have three points: $f(a)$, $f(b)$, and the middle point $f(m)$. Then, we find a quadratic function that goes through the same points. We only need to integrate the quadratic over the interval for the internal. It turns out that the integral would be,

$$\frac{b-a}{6}(f(a)+4f(m)+f(b)) \tag{1}$$

A general form based on Simpson's method would be,

$$\frac{1}{3}h[f(a)+f(b)+4\sum_{odd\ k} f(a+kh)+2\sum_{even\ k} f(a+kh)] \tag{2}$$

Based on this method, I choose my function as,

$$x^3+2x^2 \tag{3}$$

According to calculus, the exact integral would be,

$$\frac{1}{4}x^4+\frac{2}{3}x^3 \tag{4}$$

1.2. Pseudocode

The basic idea here is that we use both Simpson's and the normal calculus methods and then compare them. As always, the first thing to do is import all necessary libraries. Then, we define the Simpson method by employing some loops to achieve alternating even and odd summation as shown in equation 2. Then we define our function x^3+2x^2. After this, we set several upper limits and run a loop to perform integration over different ranges. We collect the data and compare the exact value using the calculus method. Figure 1 shows complete logic for the code.

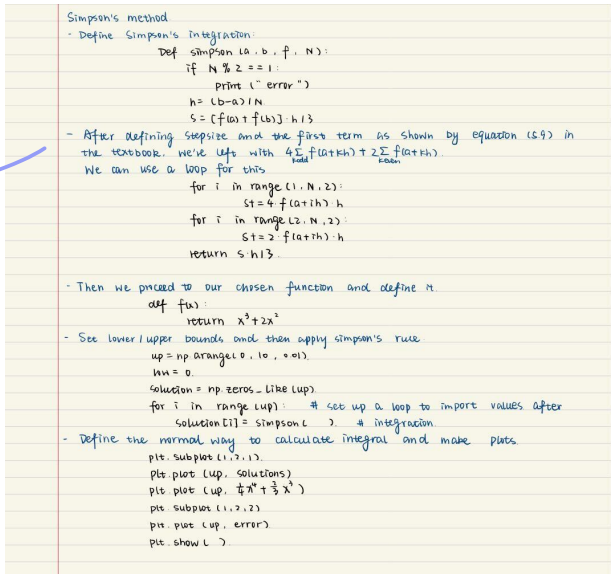

FIG. 1: [Simpson method pseudocode]

1.3. Result

Figure 2 shows the result we get using the Simpson (blue curve) and normal calculus methods (orange curve). The orange curve and blue curve cover each other, indicating a very good approximation of the Simpson method. The right plot shows the error based on a log scale, which is quite tiny on the 10^{-13} scale.

1.4. Conclusion

By setting, Simpson's method employs quadratic to make approximation. If our choice happened to be a quadratic function, then the method should show a very good fit. As shown in our plots, the error is very tiny, indicating an accurate approximation.

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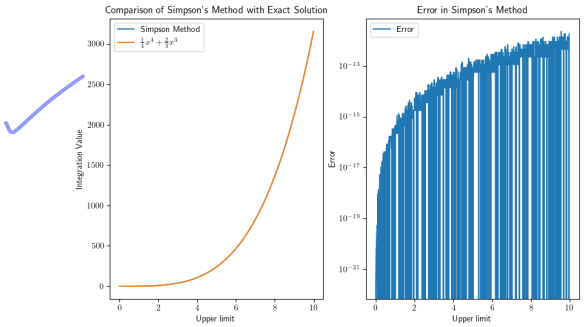

FIG. 2: [Simpson integral over equation 3]

2. QUANTUM HARMONIC OSCILLATOR

2.1. Hermite Polynomials

In this problem, we are given a wave function involving energy state, carried by the denominator and the Hermite function. In part a, we will make a plot of the Hermit function, which is described as,

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{5}$$

with $H_0(x) = 1$ and $H_1(x) = 2x$.

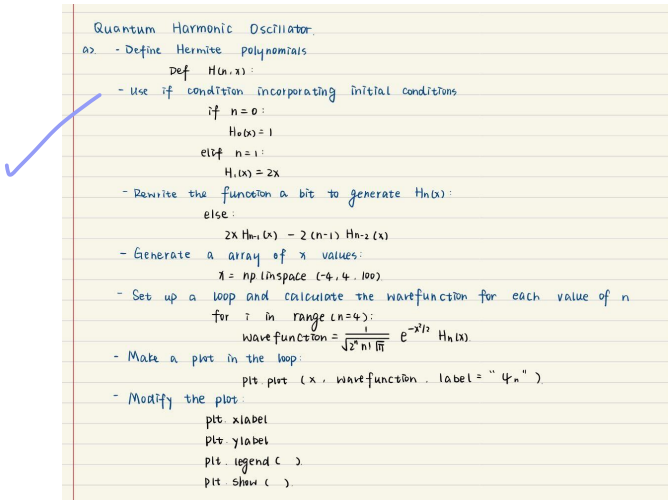

FIG. 3: [Pseudocode for part a]

Figure 3 shows the Pseudocode for part a. When defining the Hermite polynomials, I use an if condition to set up the first two orders of polynomials. Then, the loop is used to evaluate the first four orders from $n = 0$ to $n = 3$. The plot is shown in Figure 4. Based on the plot, we observe that even and odd order gives alternating symmetrical properties around $x = 0$. This is an essential polynomial that can be used to create symmetries when encountering various potential walls.

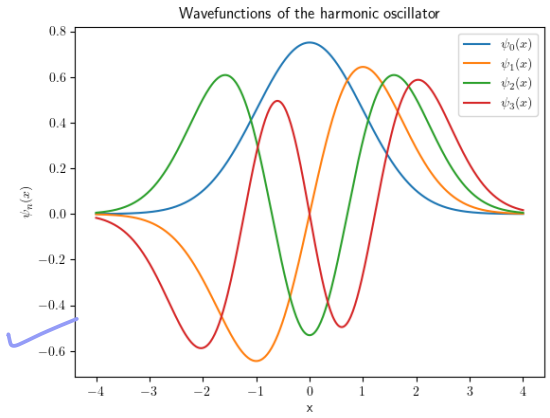

FIG. 4: [First 4 order of Hermite Polynomials]

2.2. $30th$ Polynomials

We use the code in the previous part and eliminate the loop part for this part. Set $n = 30$, then do the evaluation, as shown in Figure 5

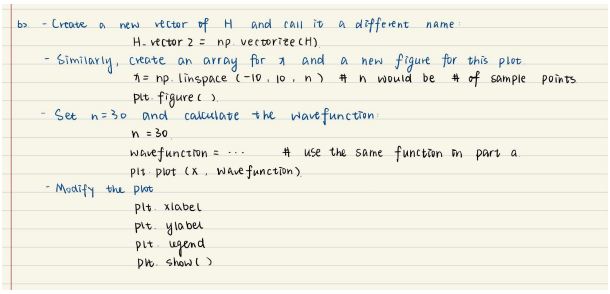

FIG. 5: [Pseudocode for part b]

And as expected, there will be 31 peaks as shown in figure 6.

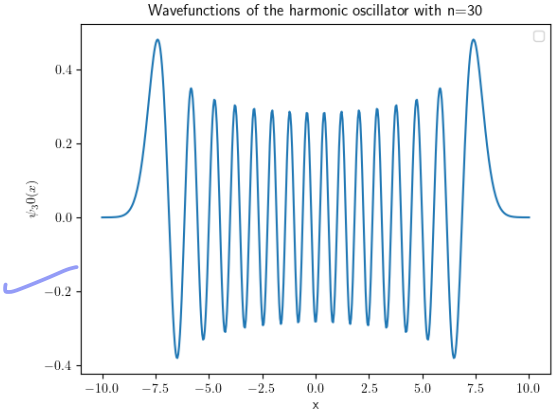

FIG. 6: [$30th$ Hermite Polynomial]

2.3. Uncertainty approximation

As defined in Statistical mechanics and quantum mechanics, the expectation value is defined as,

$$< a >= \int_{-\infty}^{\infty} a|\psi_n^2(x)|dx \tag{6}$$

In this case, we are given the position. The uncertainty of position is,

$$< x^2 >= \int_{-\infty}^{\infty} x^2|\psi_n^2(x)|dx \tag{7}$$

This integral goes from negative infinity to positive infinity. I used $x = \tan z$ and $dx = \frac{dz}{\cos^2 z}$ to transfrom the integral from infinity to $-\pi/2$ and $\pi/2$. I use the Gaussian Quadrature to do the integral, which is defined in the book's online resource.

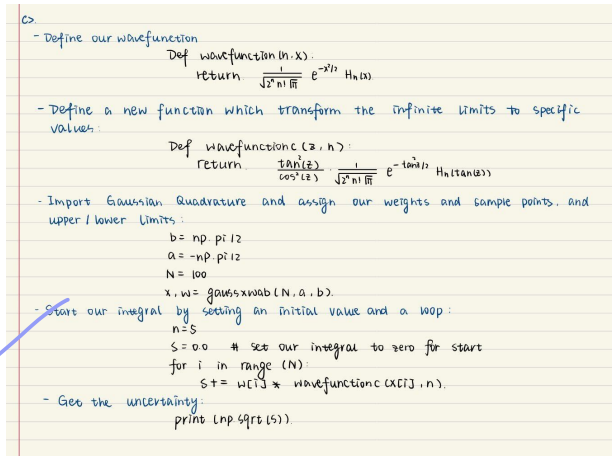

FIG. 7: [Uncertainty Approximation Pseudocode]

And I got 2.345 after taking square root of it, which agrees with the expected value.

$\sqrt{< x^2 >}$ is also called a root-mean-square deviation, which is a measure of accuracy. It also help define the width of the distribution.

2.4. Physics context

Great!

This is a one-dimensional quantum harmonic oscillator. Given a random potential around a stable equilibrium point, we can set up a Hamiltonian of the particle by,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 \tag{8}$$

The quantities with a hat above are the operators that are used a lot in quantum mechanics. $\hat{p}$ is the momentum operator and $\hat{x}$ is the position operator. Then we solve the Schrödinger equation defined as,

$$\hat{H}|\Psi >= E|\Psi > \tag{9}$$

where E is a real number showing energy. $|\Psi >$ denotes the eigenstate given a specific eigenenergy. The ψ_n given in the problem is the wavefunction formula after going through the above steps.

3. SURVEY

+5

I spent roughly 6 hours on this homework. I'm now more familiar with integration rules such as the Simpson method and Gaussian quadrature. I like the Quantum Harmonic Oscillator problem since it provides many insights into quantum mechanics. And I used tan to do the integral, which is a good practice. I think this set is about the right length.

4. UNGRADED PART

I have done all of the required and ungraded work.

Q.1

55/56

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?

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

. 6.1. Is the code author named? name? -1

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

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

9. Write-up (up to 28 points)

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

✓ . 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)

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)

2. Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)
1. Are collaborators clearly acknowledged? (+1 point)
2. Are any outside references appropriately cited? (+2 point)

5.13 55/56

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