PHYS H304 Homework 5

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This is the lab report write-up of the approach and methods used for the fourth problem set in PHYS H304.

1. INTRODUCTION

This is a summary of the methods and major equations used for this problem set. In this report, we explore methods of numerical integration, focusing largely on the application of Gaussian Quadrature and errors on approximations of integration methods. We present the plots we produced representing the evaluation of integrals of various functions and error on the integral approximation for various widths and slices used in the approximation. The major equations used are included where appropriate and a summary of the approach used to develop the code is included as well. All equations are taken from Computational Physics by Mark Newman [1].

2. METHODS

2.1. Exercise 1

For Exercise 5.3, we estimated the integral of the function given in Eqn. 1 using Simpson's rule yields a more accurate value. To evaluate Simpson's rule, we use Equation 5.10 from [1], reproduced in our Eqn. [**?**].

$$E(x) = \int_0^x e^{-t^2} dt \tag{1}$$

$$I(a,b) \cong \frac{h}{3}[f(a) + f(b) + 4\sum_{1}^{N/2} f(a + (2k-1)h) + 2\sum_{1}^{N/2-1} f(a+2kh)] \tag{2}$$

To determine the number of slices, N, that achieved a precision of 10^{-3}, we made a logarithmic scale plot of the error on the integral approximation using Simpson's rule of Eq. 1 at a fixed value of x=2 for a range of N from 1-100. The error was determined by using inspection of relative convergence as discussed in the lecture notes shown in Eq. 5 where $E(x)_N$ is the approximation of the integral for a given number of slices and $E(x)_{2N}$ is the approximation using twice the current number of slices.

$$E_{simpson} = \frac{E(x)_{2N} - E(x)_N}{E(x)_N} \tag{3}$$

To solve the integral using Gaussian quadrature, we use the python function defined by cite [1] titled gaussxw.py, wherein the integral is approximated using Equation 4. Here, wk refers to the weights determined in the intermediate steps of Gaussian quadrature and f(xk') is the integrand evaluated at the sample point x_k.

$$\int_a^b f(x)dx \cong \sum_{k=1}^{n} w_{k'} f(x'_k) \tag{4}$$

For the estimate of the error on the Gaussian quadrature approximation, we implement the same method, where we use the description in [1] that shows that the approximation of the integral for the value of 'N' that is one more than the current value can be treated as exact. Hence, the absolute error is given by the magnitude of the difference between the two estimations. In order to make a comparison to the error plotted for Simpson's rule, we take the fractional/relative error by dividing absolute error by the current approximation and treat the exact value as the approximation of the Gaussian quadrature using twice the number of sample points (i.e. 2N)

$$E_{gauss} = \frac{E(x)_{2N} - E(x)_N}{E(x)_N} \tag{5}$$

We estimate the error scales on the logarithmic plots of error as a function of N for both methods (Gaussian and Simpson), and comment on the relative accuracy of each method.

2.2. Exercise 5.13

From Smith [2], periodic oscillations that set up standing waves can be described as a set of standing waves. At points where the standing waves undergo complete destructive interference, the wave function is characterized by nodes. [2] The number of nodes, n, corresponds to the order of the harmonic. In quantum mechanics, harmonics are applicable to describe the quantization of energy, as the energy of a particle in a specific potential well is represented by a set of nth order harmonics. [3]. These set of energy wave functions are given by multiples of a set of Legendre, or Hermite, polynomials, scaled by an appropriate factor as shown in Eq. 6, where $H_n(x)$ represents the nth order Hermite polynomial.

$$\psi_n(x) = \frac{e^{\frac{-x^2}{2}}}{\sqrt{2^n n! \sqrt{\pi}}} \cdot H_n(x) \tag{6}$$

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The set of Hermite polynomials are determined by a recursive relation that Newman [1] relates to the Fibonacci sequence, where the first two terms are defined as $H_0(x)=1$ and $H_1(x)=2x$, and the remaining terms are determined using Eq. 7.

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{7}$$

We define the function that determines the Hermite polynomial for a given value of 'n' in terms of x by taking these two variables as inputs. We then use the given recursive relation to determine the remaining Hermite polynomials after setting the values for the case n=0 and n=1. Multiplying each order polynomial by the prefactor of $\frac{e^{\frac{-x^2}{2}}}{\sqrt{2^n n!\sqrt{\pi}}}$ yields the wave function representing a particular energy eigenstate of the nth energy level for a given system. For the values of n=0-3, we plot the wave functions using the recursive function we define in python.

For higher order n harmonics, the recursive function becomes quite computationally expensive to run. Therefore, we instead create an array of the possible Hermite polynomials for the range of n from 0-30 and over a range of x from -10-10. In this setup, each harmonic is determined from the preceding two rows, and can be propagated at a fixed value of n for the range of x values throughout the columns. To determine the wave functions, we create an array that scales each row of the Hermite polynomial array by the appropriate prefactor.

To determine the uncertainty, we use Gaussian quadrature with a sample of 100 points to estimate the integral given in Eqn 8. As the limits of integration stretch over an infinite domain, we set our own limits of integration and try different limits to estimate whether the solution is stable. From the plot of the wave function for the n=30 harmonic, we determine that the wave function is approximately zero at the boundaries -10 and 10. Therefore, we substitute these values as our lower and upper limits respectively to obtain an estimate of the uncertainty. Evaluating the integral at limits of integration that are twice, thrice, and four times these boundaries yields a similar result; thus, we can conclude that the contributions at x¿10 and x¡-10 are negligible. The uncertainty is then determined by taking the square root of this integral approximation, as shown in Eqn. 9.

$$< x^2 >= \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 \tag{8}$$

$$\text{uncertainty} = \sqrt{< x^2 >} \tag{9}$$

3. RESULTS AND CONCLUSION

For Exercise 5.3, in part 'a', we develop the function to evaluate the integral of the given expression for a range of values for x from 0-3. The integral approximations for this range of x using the two different methods are shown in Figure 1. At a fixed value of x=1, we plotted the error on the Gaussian approximation and that of Simpson for for various values of N. The logarithmic scale plot of these error as a function of N is shown in Figure 2.

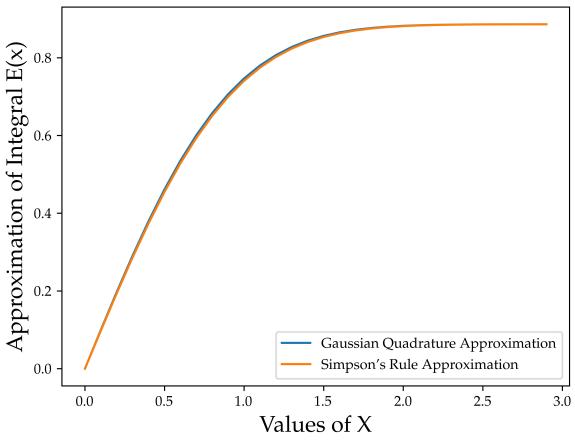

FIG. 1: A plot of the integral approximation for the range x=0-3 for two different methods of numerical integration. While the approximations are close, there is slightly noticeable difference between the two curves.

From the slope in Figure 2, we observe that the envelope linear approximation of Simpson's rule has a slope of 3. This is in accordance with Newman's description of Simpson's rule as having a cubic error [1]. In contrast, the error on the Gaussian approximation does not appear to have a linear behavior. Rather, the slope is much steeper and is continuously changing, showing a dependency on the number of slices N. As discussed in class, Gaussian quadrature converges to the exact solution very quickly, on the order of N^{-N}, indicating its higher level of accuracy. This can be observed in the plot where at values of N> 10, the error on Gaussian quadrature exceeds machine epsilon (10^{-16}), and then shows random behavior that reflects error due to the limitations of the machine. Hence, Gaussian quadrature converges at a much faster rate than Simpson's rule approximations, and in a non-linear manner.

For Exercise 5.13 a, we observe the expected harmonics relationship for the first four wave functions. For the initial standing wave, n=0, there are no observed nodes. For the harmonic n=3, we observe three nodes in Figure 3. For the harmonic n=30, we observe thirty nodes, as shown in Figure 4. Hence, the expected relationship between harmonics is observed for the energy eigenstates of the quantum harmonic oscillator. Using Eqn 8, we are able to estimate that the uncertainty in the position for the n=5 harmonic oscillator is 2.34 to

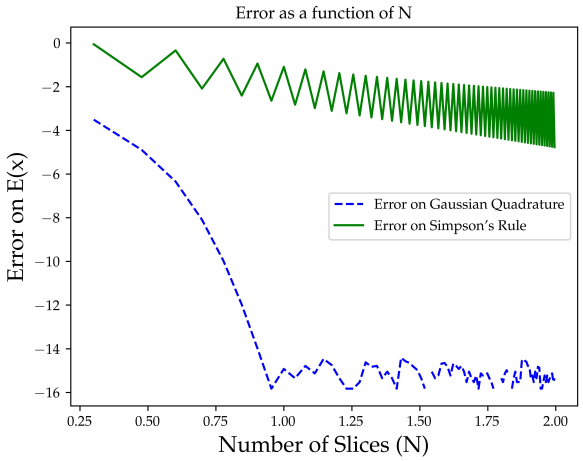

FIG. 2: A plot of the error as a function of N for a fixed value of x=1 for the two different methods of numerical integration. Gaussian quadrature converges faster and is hence more accurate.

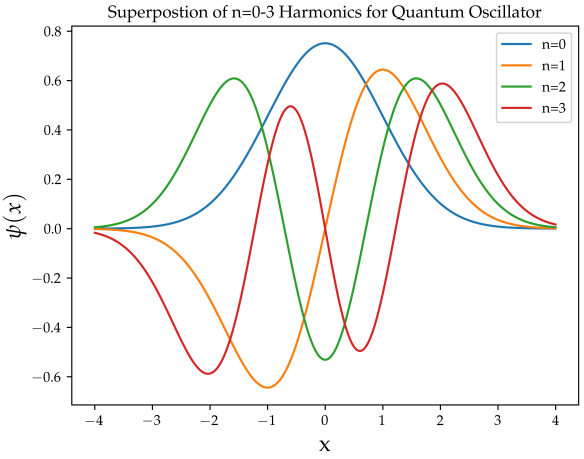

FIG. 3: A plot of the harmonics for the quantum oscillator for the energy levels of n=0, n=1, n=2, n=3.

three significant figures. See python code attached for further information.

4. SURVEY QUESTION

The most interesting problem was 5.13. The homework took me about 10 hours to complete. I learnt how to apply the coding we have been learning to practical concepts in Physics, particularly in quantum mechanics, and apply numerical integration. I think the problem set length and difficulty were just right, although I think the instructions and caution against using recursive functions could have been elaborated upon further for Exercise 5.13.

[1] M. Newman, *Computational Physics* ([Createspace], 2012), URL http://www-personal.umich.edu/~mejn/cp/index.html.

[2] W. F. Smith, *Waves and Oscillations: A Prelude to Quantum Mechanics* ([Oxford University Press], 2010).

[3] J. S. Townsend, *Quantum Physics: A Fundamental Approach to Modern Physics* ([University Science Books], 2010).

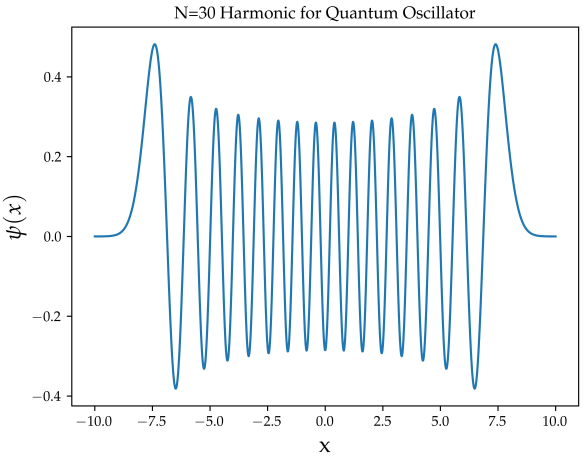

FIG. 4: A plot of the harmonic oscillatore for the level n=30.