Phys 304: Homework 5

Mary Smith*
Haverford College Department of Physics
(Dated: March 8, 2024)

[The homework took me about 10 hours this week. I learned about the nature of Gaussian quadrature and to be careful when using it that it is being used with a polynomial. The most interesting problem was the quantum uncertainty in the harmonic oscillator because it was so challenging. The problem set was just the right length. My collaborator for this problem set was Luke Smithberg.]

1. PROBLEM 1: SIMPSON INTEGRATION

Simpson's rule is a modified and much more accurate version of the trapezoidal approximation of a function. It gives an approximation to the area under two adjacent slices of a function. The application to the area under a function involves the height of the slices and values of the function at evenly spaced values. In formula version, this is given by

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

where N is the number of slices, $f(x)$ is the function being integrated over, a and b are the bounds of integration, h is $h = \frac{b-a}{N}$, and k is the index of summation.

1.1. Coding Simpson's rule

In order to create the code to use Simpson's rule to approximate the integral of a function, the process outlined in Figure 1 was followed. In this method, we broke the sums into two different for loops and evaluated the function over the for loops. These were then evaluated as the total approximation of the integral. The integral $\int_0^{10} x^2 dx$ was evaluated using the approximation, resulting in a value of 333.333.

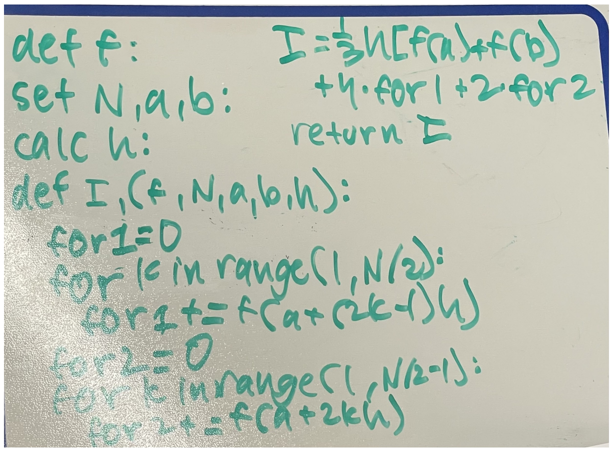


FIG. 1: [The pseudocode to approximation an integral using Simpson's rule.]

2. PROBLEM 2: QUANTUM UNCERTAINTY IN THE HARMONIC OSCILLATOR

A spinless point particle in a quadratic potential well can be modelled as a one-dimensional quantum harmonic oscillator. In units where all the constants are 1, the wavefunction of the nth energy level of the one-dimensional quantum harmonic oscillator is given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} e^{\frac{-x^2}{2}} H_n(x) \quad (2)$$

for $n = 0, 1, 2, ...\infty$, where $H_n(x)$ is the nth Hermite polynomial. The Hermite polynomial is given by

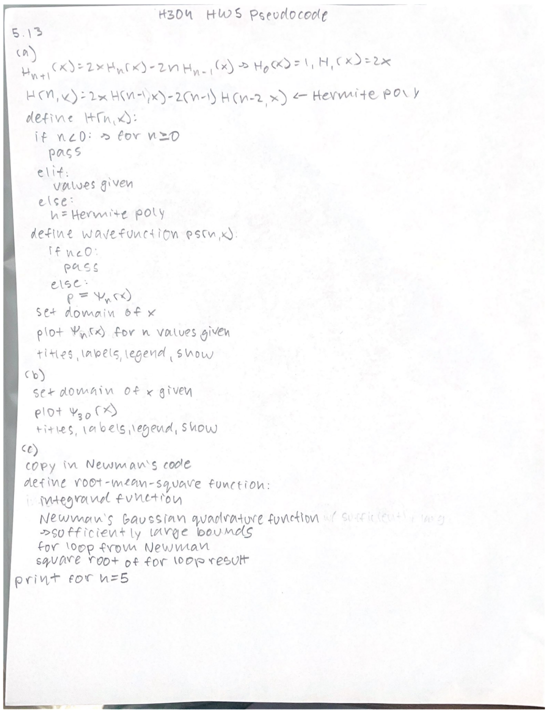
$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x), \quad (3)$$

where the first two Hermite polynomials are $H_0(x) = 1$ and $H_1(x) = 2x$. The psuedocode for this problem can be found in Figure 2.

2.1. Part (a): Plot of harmonic oscillator wavefunctions for varying n

A user defined function H(n,x) was created to calculate the Hermite polynomial in Eq. 3 for given x and any integer $n \geq 0$, using recursion. The Hermite polynomial was then plugged into the wavefunction in Eq 2 to create a user defined function ps(n,x). This was then used to create a plot that shows the harmonic oscillator wavefunctions for n=0,1,2, and 3 on the same graph in the range x=-4 to x=4. This graph can be seen in Figure 3. The figure shows how the number of nodes of a particle in a potential well various with the number n.

*Electronic address: masmith@haverford.edu



```
H304 HW5 Pseudocode
5.13
(a)
H_{n+1}(x)=2xH_n(x)-2nH_{n-1}(x) -> H_0(x)=1, H_1(x)=2x
H(n,x)=2xH(n-1,x)-2(n-1)H(n-2,x) <- Hermite poly
define H(n,x):
  if n<0: -> for n≥0
    pass
  elif:
    values given
  else:
    h=Hermite poly
define wavefunction ps(n,x):
  if n<0:
    pass
  else:
    p = ψ_n(x)
set domain of x
plot ψ_n(x) for n values given
titles, labels, legend, show
(b)
set domain of x given
plot ψ_30(x)
titles, labels, legend, show
(c)
copy in Newman's code
define root-mean-square function:
  integrand function
  Newman's Gaussian quadrature function
  ->sufficiently large bounds
  for loop from Newman
  square root of for loop result
print for n=5
```

FIG. 2: [The pseudocode for the quantum uncertainty in the harmonic oscillator.]

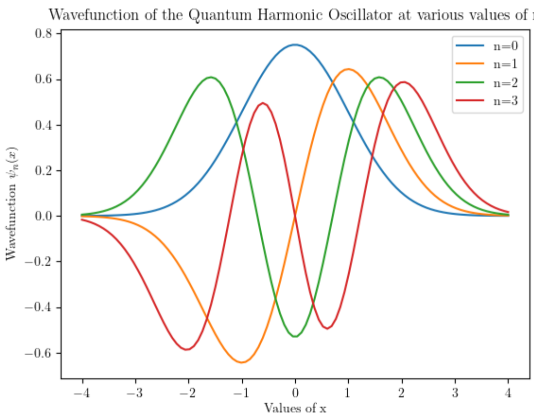


FIG. 3: [A plot showing the harmonic oscillator wavefunctions at various given values of n, in range x=-4 to x=4.]

2.2. Part (c): Plot of the harmonic oscillator wavefunction at value of n

The user defined function for the wavefunction of the harmonic oscillator derived in Sec. 2.1 was used to create a plot for the harmonic oscillator wavefunction at n=30 over the range x=-10 to x=10. The method for this is highlighted in Figre 2. The plot for this wavefunction is included in Figure 4. The plot shows an interesting behavior for an increased value for n.

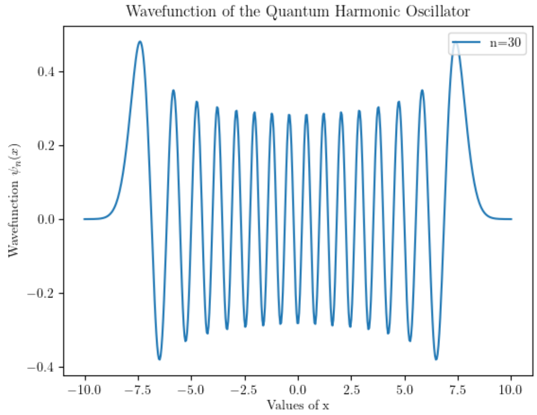


FIG. 4: [A plot showing the harmonic oscillator wavefunction at n=30, in range x=-10 to x=10.]

2.3. Part (c): The quantum uncertainty

The quantum uncertainty in the position of a particle in the nth level of a harmonic oscillator can be quantified by its root-mean-square position $\sqrt{\langle x^2 \rangle}$, where

$$\langle x^2 \rangle = \int_{\infty}^{\infty} x^2 |\psi_n(x)|^2 dx. \tag{4}$$

A program was written to evaluate this integral using Mark Newman's Gaussian quadrature on 100 points, and then calculate the uncertainty for a given value of x. The program was used to calculate the uncertainty for n=5, about 2.3. However, I encountered something very interesting when running the Gaussian quadrature equation. Because I was using a very large domain in order to accurately model an integration over infinity, I was adding up a lot of very small numbers because of the nature of the integrand. The integrand is not a polynomial, so care must be taken with the domain and the number of points. In order to get an uncertainty close to what was expected, I had to integrate from x=-10 to x=10. If I integrated over a large domain like x=-1000 to x=1000, my uncertainty was 0 because the integrand was not a polynomial.