Ps 4 Problem 3

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Abstract

This short paper will show some plots about the quantum harmonic oscillator and show a comparison between Gauss-Legendre and Gauss-Hermite quadrature for integrating the same function.

1 Introduction

The quantum harmonic oscillator wave function is a pretty well known function in quantum mechanics. Here I plot them for n = 1,2,3,4, and 30. I then calculate the variance, $< x^2 >$, for the n = 5 case in two different ways. The equation for the quantum harmonic oscillator is as follows:

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

H_n is the nth Hermite polynomial which is recursively defined as follows:

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

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

2 Methods

I began by creating a recursive function of the Hermite polynomials and then defining a psi function that includes that and plotting psi for various n. See fig 1 and fig 2 below. Next we were to look at the second moment of psi over all of space aka $< x^2 >$ which is given by:

$$< x^2 > = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 dx \tag{3}$$

This integral was done using Gauss-Legendre quadrature and then done using Gauss-Hermite quadrature. Gauss-Hermite can be done directly with slight modifications of psi, but Gauss-Legendre required a change of variables because it is only for integrals between -1 and 1. This was done for n = 5 for psi.

3 Results

The psi plots are as you'd expect although you don't normally go to n = 30 by hand because it would talke a long time. Both quadratures gave the expected value of about 2.345, but the Legendre quadrature requires upwards of 100 points to be very accurate while Hermite quadrature only needs 7 points before it no longer updates its value.

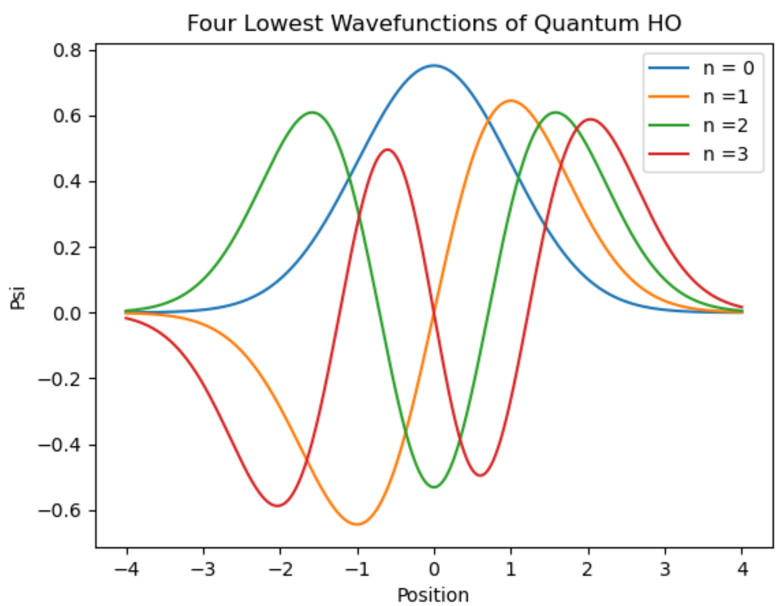

Figure 1: Plots of Psi for different energy levels.

4 Discussion

Choosing the right type of quadrature is very important for accuracy in integration. I didn't show it but even at 100 points the Legendre quadrature is still over and then underestimating the correct value. Hermite quadrature is the better form because it doesn't require a change of variables away from infinity that doesn't always fully capture the behavior. The psi function is just a polynomial when you remove the exponential so Hermite quadrature should be able to give you the exact answer to within overflow errors margin.

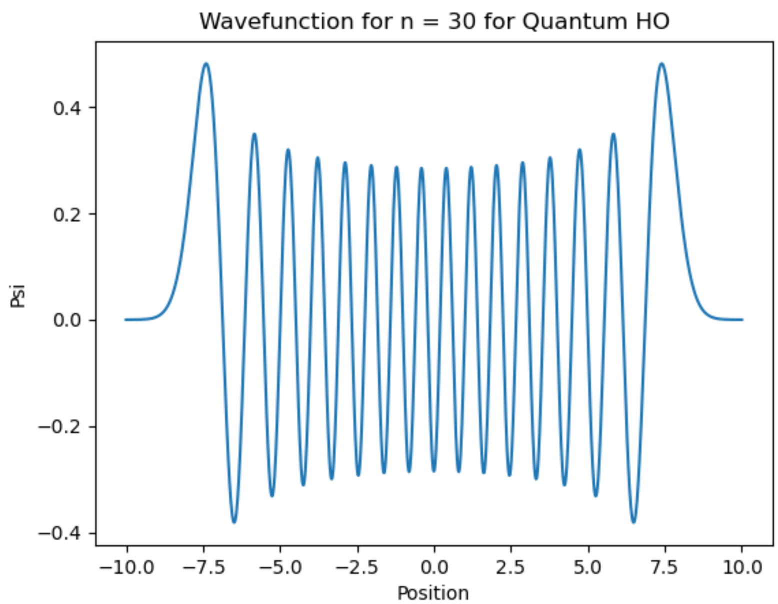

Figure 2: Plot of psi for the n = 30 energy level. There are 31 max/mins as you would expect.

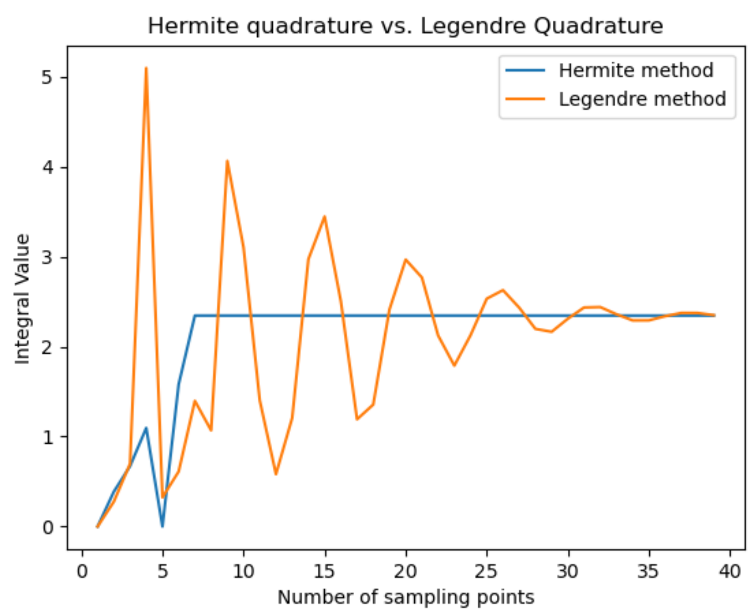

Figure 3: Gauss-Hermite is the better method and requires far fewer points to decide on an answer, but if you give enough points Gauss-Legendre also works.