Problem Set 4

By Hayden Orth; GitHub: haydenorth

October 3, 2023

Abstract

This article contains my solutions to Problem Set 4 for the graduate Computational Physics course. Problem Set 3 investigates numerical methods for integration. Also I apologize that the figures are scattered throughout the report. I tried to get them to behave but they just wouldn't.

1 Problem 1: Heat Capacity of a Solid

Problem 1 investigates using Debye's theory of solids to calculate a solid's heat capacity. This involves using the computer to evaluate an integral. To calculate the heat capacity for a given temperature, I created a function for the integrand, a function to calculate the integral using Gaussian quadrature, and a function that calls the previous function and multiplies the integral by the necessary constants to acquire the heat capacity (Cv function). I used Mark Newman's gaussxw module to get the sample points and weights for the Gaussian quadrature calculation. My Cv function takes the temperature T and the number of sample points N as arguments. Thus I can easily see the dependence of Cv on T by iterating through T values and calling the function (Figure 1). The same procedure works for testing the how the integral converges as the number of sample points, N, varies (Figure 2). According to Figure 2, 10 sample points was enough for the calculation to converge to a value, because increasing N had no effect on the calculated Cv value.

2 Problem 2: Period of an Anharmonic Oscillator

In problem 2, I study the dependence of the period of an anharmonic oscillator on its oscillation amplitude. We can invert a function of the oscillator's energy to give a differential equation in dx/dt as follows.

$$E = \frac{1}{2}m(\frac{dx}{dt})^2 + V(x)$$

$$\sqrt{\frac{2}{m}(V(a) - V(x))} = \frac{dx}{dt}$$

$$t = \int_0^a \frac{dx}{\sqrt{\frac{2}{m}(V(a) - V(x))}}$$

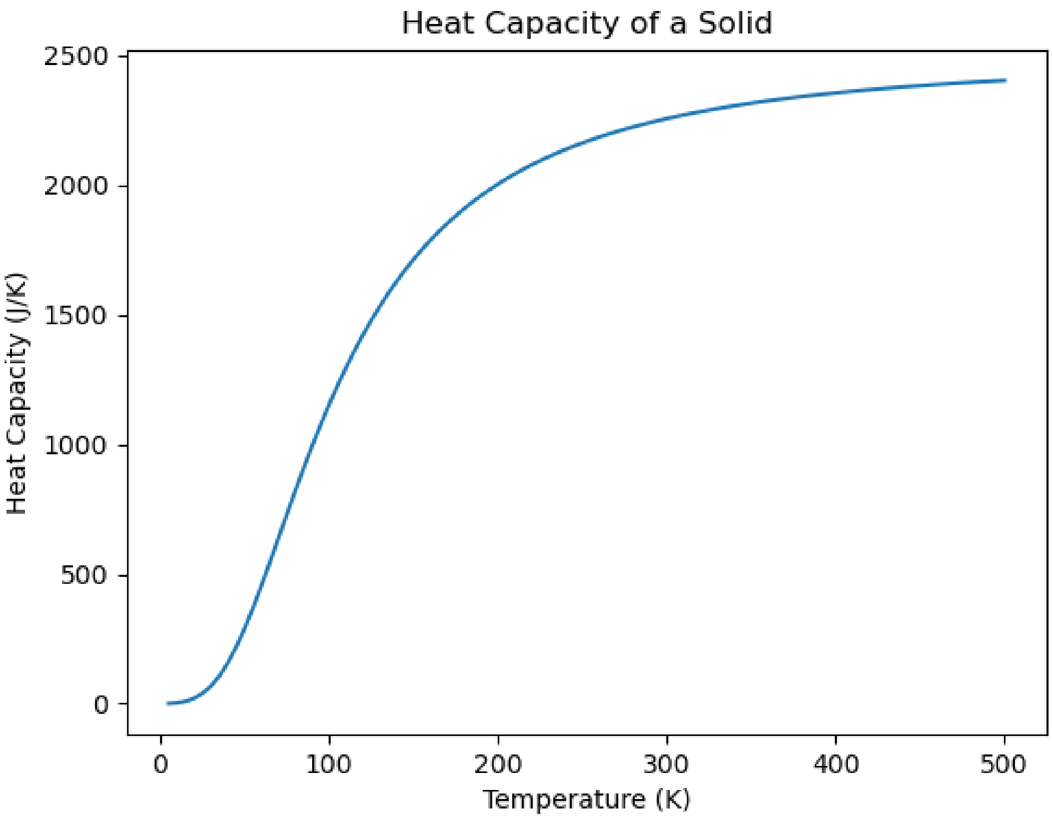

Figure 1: Problem 1 Data. Calculated heat capacity values versus temperature.

But this t corresponds to motion from the greatest amplitude down to $x = 0$, so it corresponds to a quarter of a period. Thus the period is four times the above integral:

$$T = \sqrt{8m} \int_0^a \frac{dx}{\sqrt{(V(a) - V(x))}}$$

Thus, solving for the period of the oscillator involves calculating an integral. I calculated this integral using a Gaussian quadrature procedure similar to Problem 1. In this case, I created a function get_T that takes the oscillator's amplitude and returns its period by calculating the above integral via Gaussian quadrature. I then calculated the period over 50 amplitude values between 0 and 2. The period decreases as the oscillation amplitude increases. As the amplitude goes to zero, the period diverges. This can be explained by the shape of the potential $V(x) = x^4$. x^4 is flat near x = 0 and increases steeply as x moves away from zero. Since V increases steeply, it makes sense that the period decreases as the amplitude increases. For amplitudes near zero, the potential is nearly flat, so it makes sense that the period diverges. When the potential is very flat, the oscillator will move slowly. An amplitude of zero would correspond to the oscillator not moving at all, or a period of infinity.

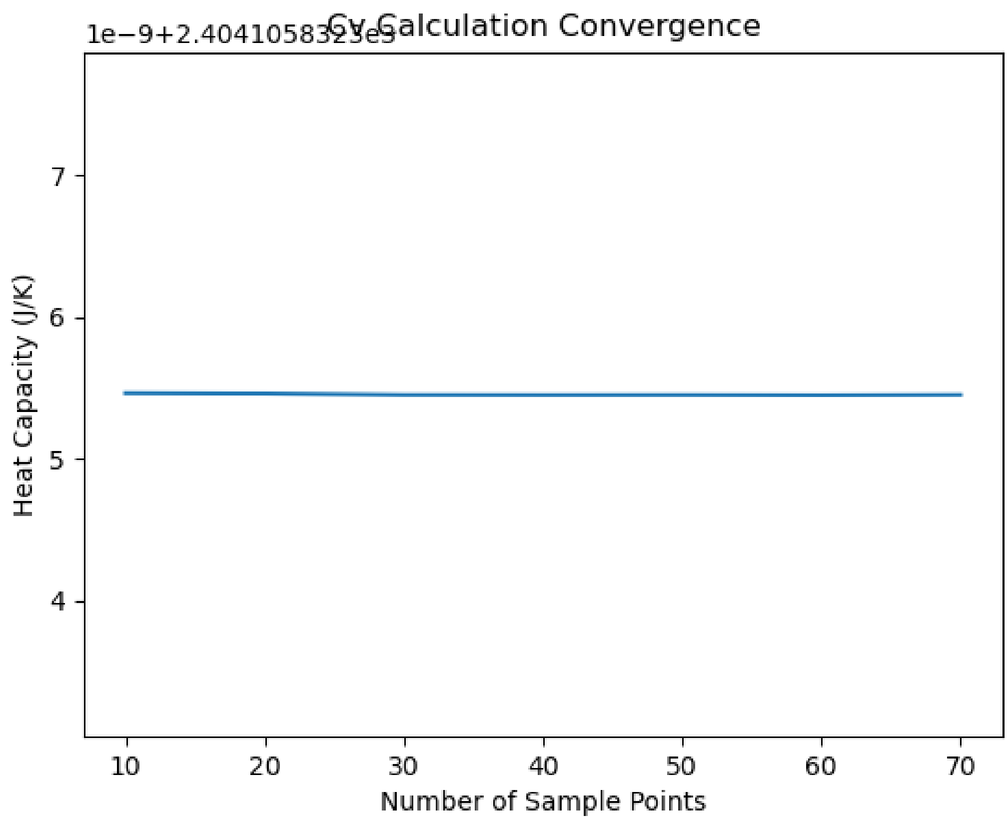

Figure 2: Problem 1 Data. Calculated heat capacity value for 500 K as a function of the number of Gaussian quadrature sample points.

3 Problem 3: Quantum Uncertainty in the Harmonic Oscillator

Problem 3 is an investigation into the wavefunction of the harmonic oscillator and quantum uncertainty in the harmonic oscillator. I created a recursive function for the Hermite polynomials and a function for the wavefunction Psi. I use this function to plot the wavefunctions for n = 0, 1, 2, 3 and n = 30 (part b). Part c involves calculating the quantum uncertainty of the oscillator via the root mean square of its position. This involves integrating the wavefunction. I evaluated this integral with Gaussian quadrature in a procedure similar to the previous two problems. The difference here is that the integral needed to be evaluated from negative infinity to infinity. To do this, I needed to change variables and evaluate the integral from -1 to 1. The program returned an rms position value of 2.3, which was the correct value. In part d, I used Gauss-Hermite quadrature to evaluate the integral. The procedure is similar to that of Gaussian quadrature, but I used scipy.special's roots_hermite function to generate the sample points and weights. I also removed the exponential term from the function for psi, as the exponential term is built into

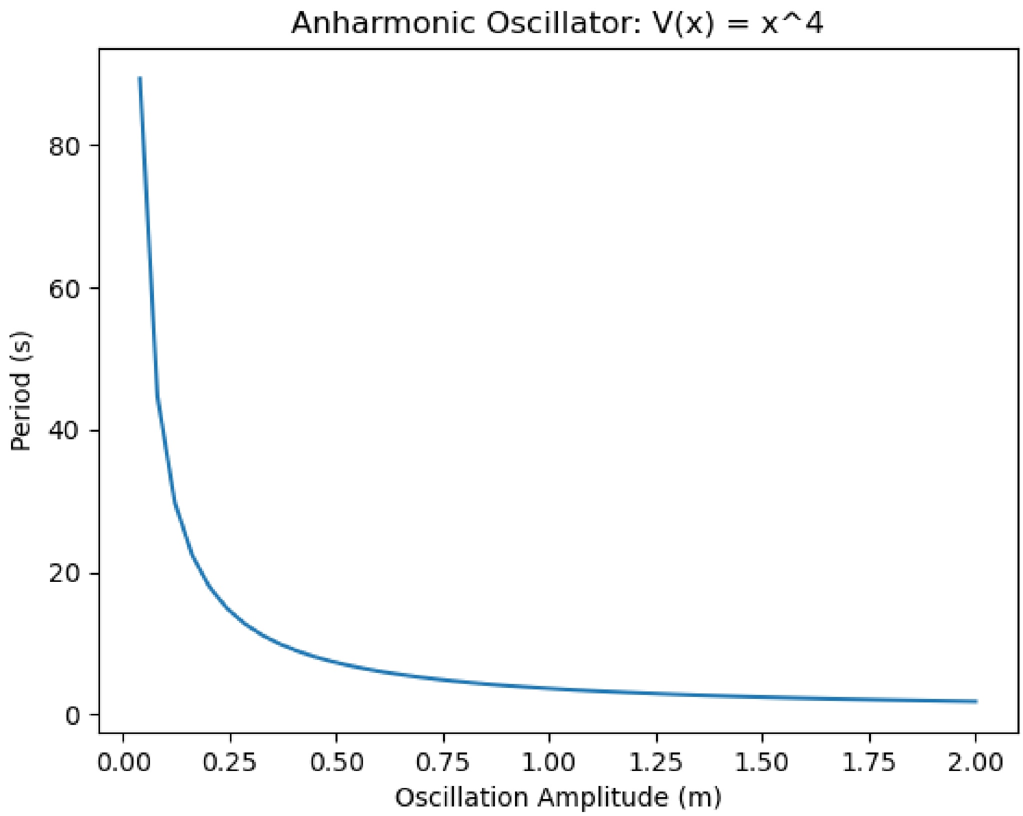

Figure 3: Problem 2 Data. Plot of oscillator periods as a function of oscillator amplitude for $V(x) = x^4$.

the Gauss-Hermite quadrature evaluation. I believe that I can make an exact evaluation of the integral. Since the sample points of the Gauss-Hermite method are the roots of the N^{th} degree Hermite polynomial, using 100 sample points will correctly integrate the wavefunction for n=5, since the n=5 wavefunction involves a 5th order polynomial. The function we are interested in integrating is of much lower order than the Hermite polynomials used in the integration, so the integration will be exact.

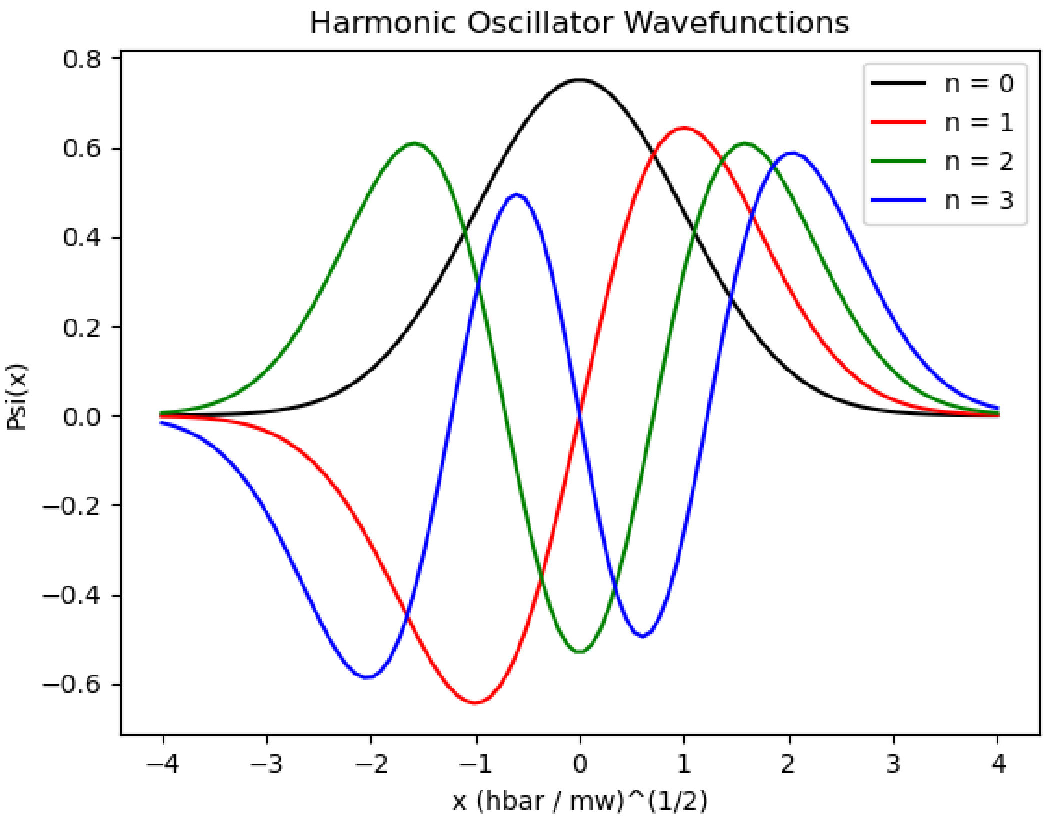

Figure 4: Plot of the first four wavefunctions of the harmonic oscillator.

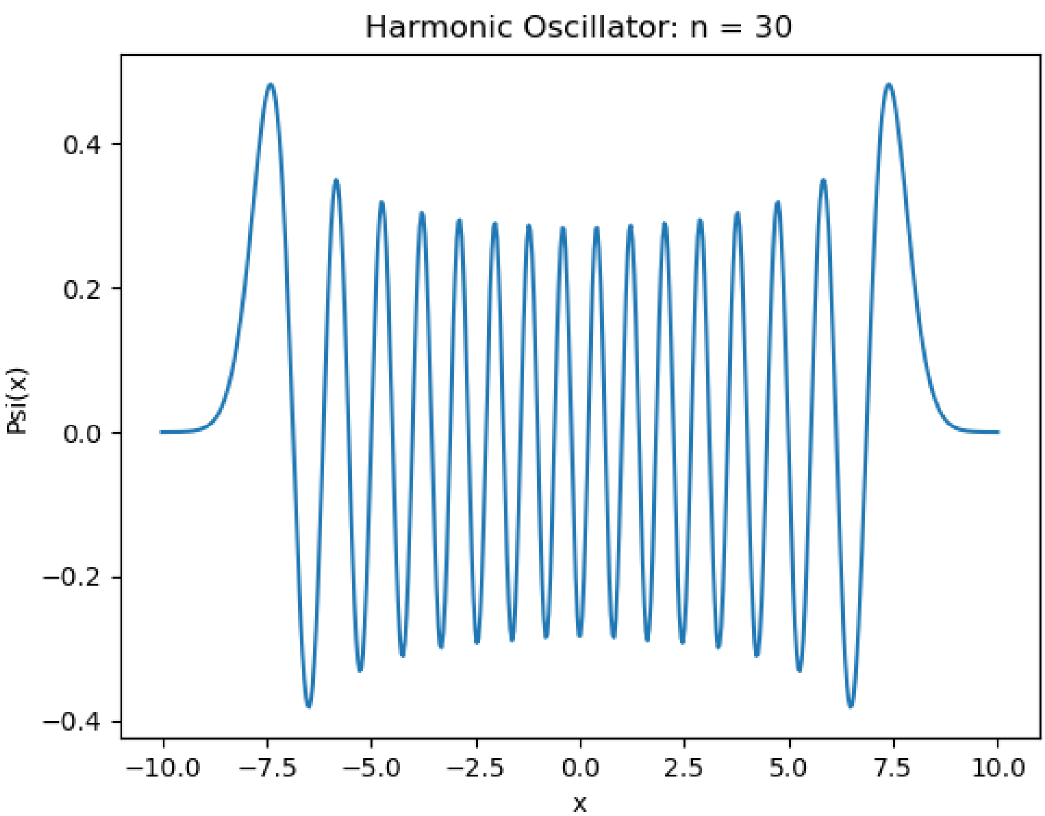

Figure 5: Plot of the harmonic oscillator wavefunction for n = 30.