Problem Set 4

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1 Finding Specific Heat Capacity with Gaussian Quadrature

The specific heat capacity of a solid is given by the following formula:

$$C_v = 9V\rho k_B(\frac{T}{\theta_D})^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2}\,dx \tag{1}$$

I wrote a Python program to calculate the specific heat capacity at a given temperature for a 1000 cubic centimeter sample of aluminum using a 50 point Gaussian Quadrature. Using this program I have graphed the specific heat of this sample as a function of temperature from 5K to 500K. See figure 1 for the results.
Figure 2 tests the convergance by evaluating the specific heat capacity using varying number of gaussian points. (I used the choices N = 10, 20, 30, 40, 50, 60, 70.)

2 Period of Anharmonic Oscillator

It can be shown that the energy of an anharmonic oscillator is given by:

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

we can rearrange this equation to find an expression for the period (T):

$$\frac{dx}{dt} = \sqrt{\frac{2}{m}[V(a) - V(x)]} \tag{3}$$

$$\int_0^{\frac{T}{4}} dt = \sqrt{\frac{m}{2}} \int_0^a \frac{dx}{\sqrt{[V(a) - V(x)]}} \tag{4}$$

$$T = \sqrt{8m} \int_0^a \frac{dx}{\sqrt{[V(a) - V(x)]}} \tag{5}$$

Considering a potential well defined by

$$V(x) = x^4$$

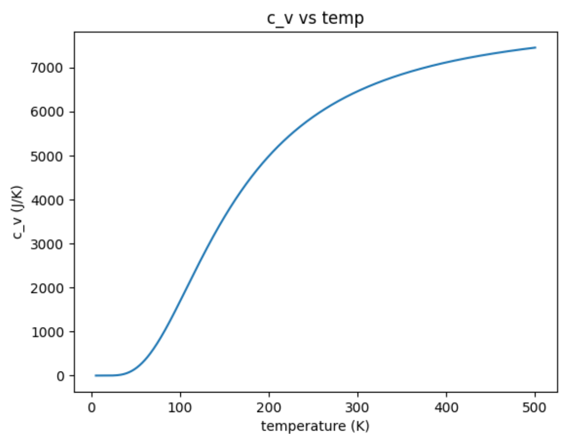

Figure 1: Specific Heat Capacity of aluminum as a function of temperature.

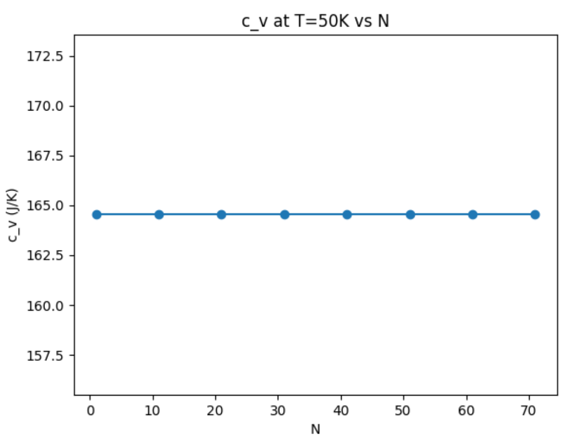

Figure 2: Here is the specific heat capacity solved at different number of points for gaussian quadrature. Its a line!

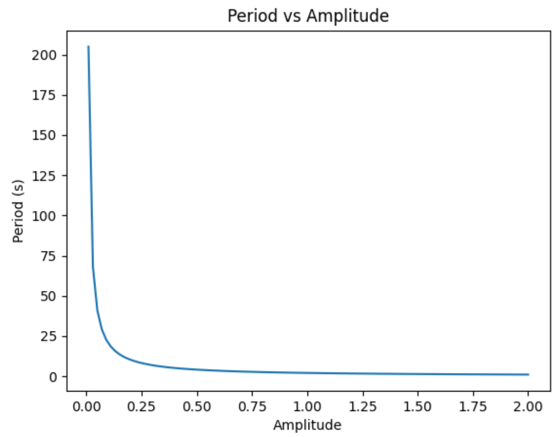

Figure 3: Period vs amplitude for anharmonic oscillator. Notice T approaches zero as Amplitude approaches 0. Also T approaches zero as amplitude increases.

I plotted the period of oscillations, T, vs the amplitude of oscillation, a from a = 0 to a = 2. See figure 3 for the results.
In the graph we see the period blows up at a = 0 and decreases as a increases. This suggests that the speed of oscillation is increasing with the amplitude. This makes sense because the restoring force of an anharmonic oscillator is not linearly related to the amplitude, instead the speed will increase more so than if it were a mere harmonic oscillator.

3 Quantum uncertainty in Harmonic Oscillator

We can easily generate hermite polynomials using an iterative python program. The Polynomials have the following form:

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{6}$$

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

These polynomials are useful for expressing the waveform of the nth energy level of a 1-d quantum harmonic oscillator. This is the expression for such a wavefunction:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n1\sqrt{\pi}}} e^{-x^2/2} H_n(x) \tag{7}$$

I plotted wavefunctions for n = 0, 1, 2, 3 as seen in figure 4. Next i plotted only the wavefunction corresponding to n=30 in figure 5

Next I calculated the uncertainty of a particles position given by the root mean square of its

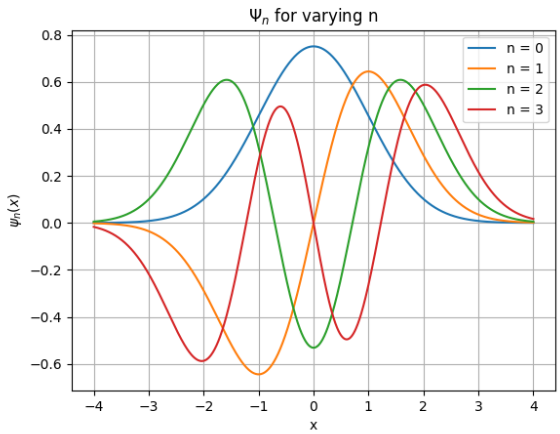

Figure 4: Here are all 4 wavefunctions plotted together for n = 0, 1, 2, 3,

position: $\sqrt{\langle x \rangle}$ where

$$\langle x \rangle = \int_{-\infty}^{\infty} x^2 |\psi_n(x)|^2 dx \tag{8}$$

Solving for this value presents a new obstacle for gaussian quadrature. We now have infinite bounds and need to use a new method of mapping our bounds. Using the transformation $x = tan(z\pi/2)$ and $dx = \frac{dz\pi/2}{cos^2(z\pi/2)}$. Using this transformation I found the RMS of the position to be: 2.34520787.

An alternative method for solving this integral is to use Hermite-Gauss quadrature. By using this method, I obtained a value of 2.345207879. I compared this to the expected value and yielded a minuscule difference on the order of 10^{-15}. We know the expected error by the following:

$$\langle x \rangle = (n + 1/2)\frac{\hbar}{m\omega} \tag{9}$$

but $m = 0, \hbar = 0, \omega = 0$ so,

$$\sqrt{\langle x \rangle} = \sqrt{(n + 1/2)} \tag{10}$$

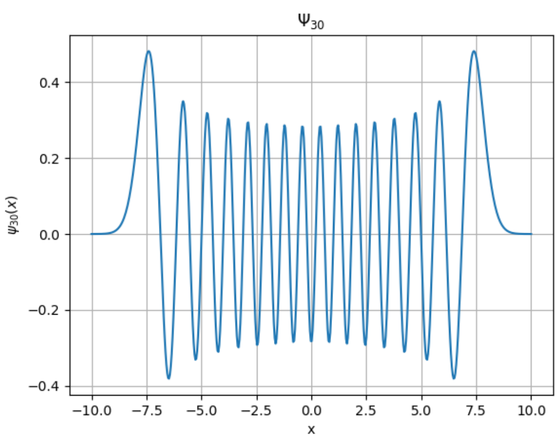

Figure 5: The wavefunction of the 30th energy level of a 1-d quantum harmonic oscillator