PS-4

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Abstract

This problem set provides practice problems on performing numerical integrals in Python. Two methods were implemented; Gaussian Quadrature and Gauss-Hermite Quadrature. Generally, the methods showed high convergence even when using a low number of sampling points. The main conclusion is that sampling methods can be useful for solving numerical integrals, but the right type of functions should be used according to the problem. Code scripts are available at `https://github.com/Leen-Alrawas/phys-ga2000/tree/main/ps-4`.

1 Solutions and Computational Methods

1. The heat capacity C_v of a solid from Debye's theorem was calculated as a function of the temperature. The integral was performed using the Gaussian Quadrature sampling method. The weights and the sampling points were calculated using the package `gaussxw`. Using $N = 50$ (number of sampling points), C_v was plotted as a function of the temperature (Figure 1).
   In part c, we vary the number of sampling points to calculate C_v while keeping the temperature constant at $T = 50K$ (Figure 2). The convergence was fast and the answer was sufficiently accurate at only $N = 7$ (Figure 3).
2. (a)

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

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

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

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

   (b) The period of an anharmonic oscillator was plotted as a function of the amplitude. See Figure 4.
   (c) We can see from the plot that the period decreases as the amplitude increases. It is true that with larger amplitudes, the particle needs more time to complete one period as the **period is proportional to the traveled distance**. However, it is also **inversely proportional to the particle's speed**. If we increase the amplitude, we give the particle

more energy which will be converted to kinetic energy. The energy of the system is constant and by the energy equation, if we increase the amplitude, the potential energy increases by a power of four ($V(x) = x^4$) and we increase the maximum speed by a power of two ($K(v) = \frac{1}{2}mv^2$) while the distance is only increased by the same order of the amplitude (power of one). Hence, the speed has a dominant effect on the period and the period decreases with increasing amplitudes. The inverse is also true; as we decrease the amplitude the particle gets slower and slower giving a diverging period at amplitudes close to zero.

3. (a) Hermite Polynomials are defined as recursive relations. The plot in Figure 5 shows the first 4 functions for $n = 0, 1, 2, 3$.
(b) Figure 6 shows $H_{30}(x)$.
(c) Using 100 sampling points, the Gaussian Quadrature method gave a result of 2.3452078737858173 for the root mean square value. The infinite integral was performed using the following variable transformation:

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-1}^{1} \frac{1+z^2}{(1-z^2)^2} f(\frac{z}{1-z^2})dz$$

(d) Because the function has a factor of e^{-x^2}, Gauss-Hermite Quadrature is more suitable for this problem as this factor will cancel out. In addition, there is no need for a variable change. Using only 10 sampling points, this method reduced the error from 10^{-7}% (in part c with 100 sampling points) to 10^{-14}% (see Figure 7). The exact solution was found to be $\sqrt{5.5}$ using Mathematica. Increasing the number of sampling points does not reduce the error anymore.

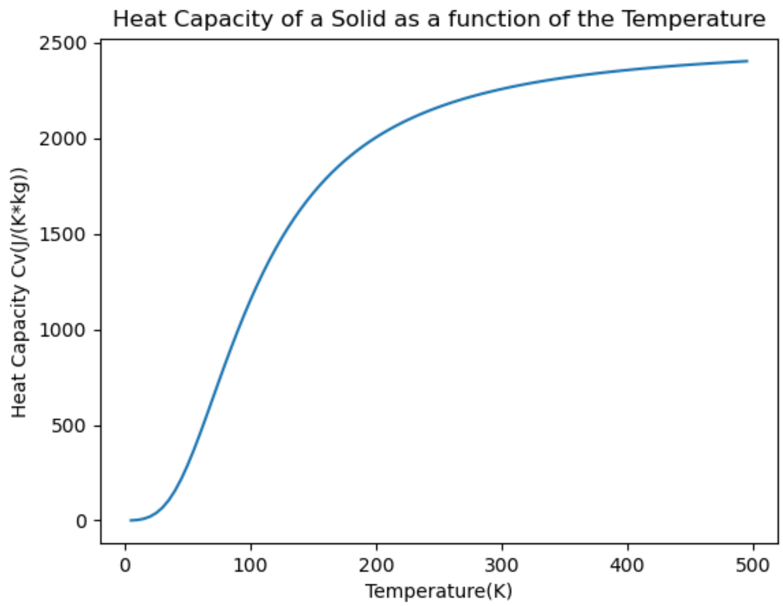

Figure 1: Heat Capacity of a solid as a function of T, with $\theta_D = 428K$, $\rho = 6.022 \times 10^{28} m^{-3}$, and $V = 1000 cm^3$.

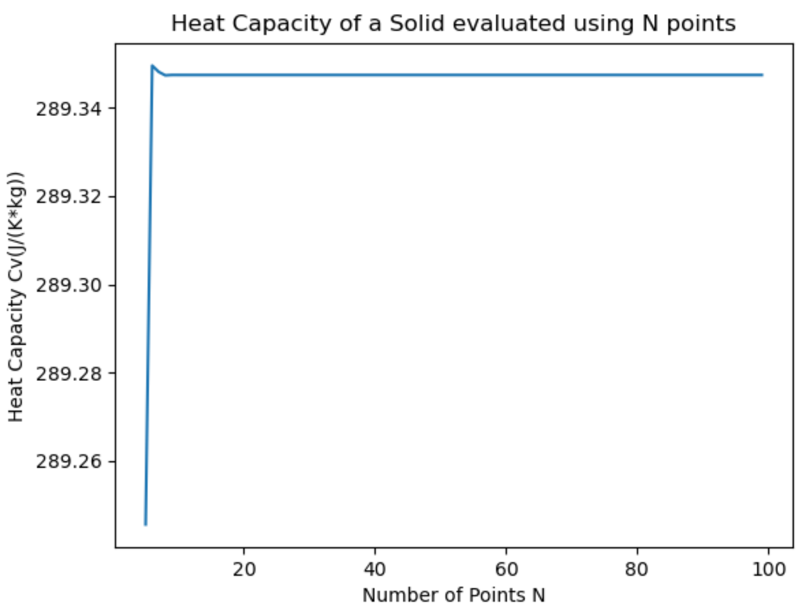

Figure 2: Heat Capacity of a solid using different number of sampling points $1 \leq N \leq 100$, with $\theta_D = 428K$, $\rho = 6.022 \times 10^{28} m^{-3}$, $T = 50K$, and $V = 1000 cm^3$.

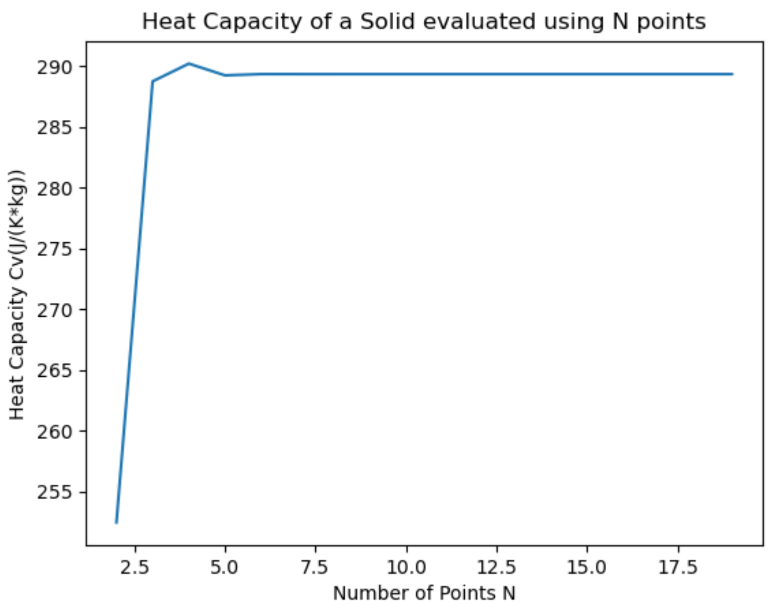

Figure 3: Heat Capacity of a solid using different number of sampling points $1 \leq N \leq 20$, with $\theta_D = 428K$, $\rho = 6.022 \times 10^{28} m^{-3}$, $T = 50K$, and $V = 1000 cm^3$.

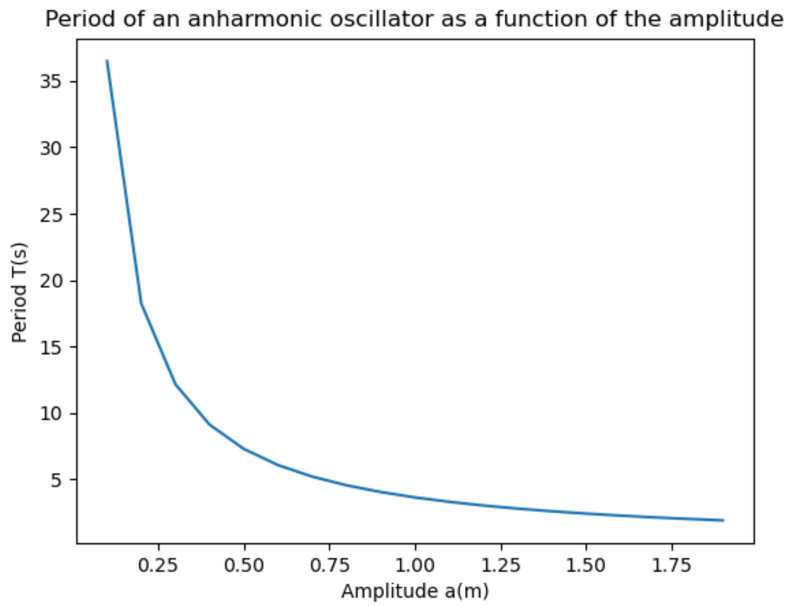

Figure 4: The period of an anharmonic oscillator for different values of the amplitude using $m = 1kg$.

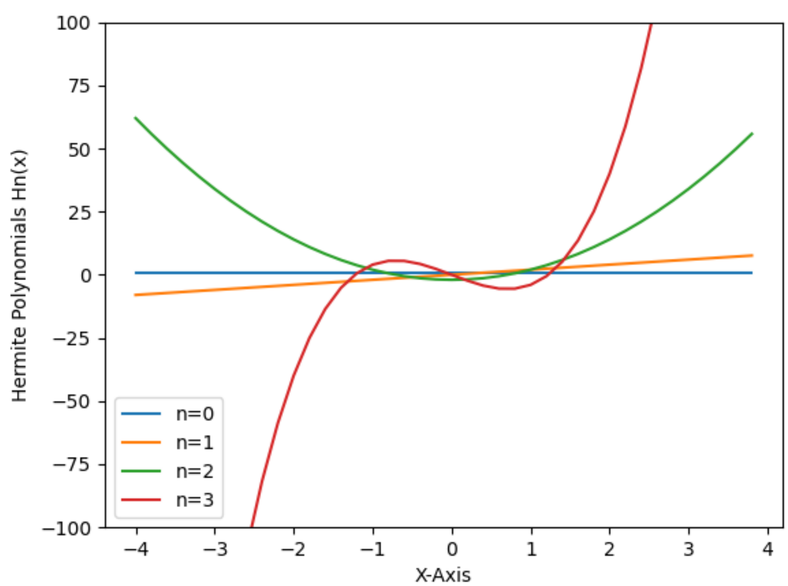

Figure 5: Hermite Polynomials $H_n(x)$ for $n = 0, 1, 2, 3$.

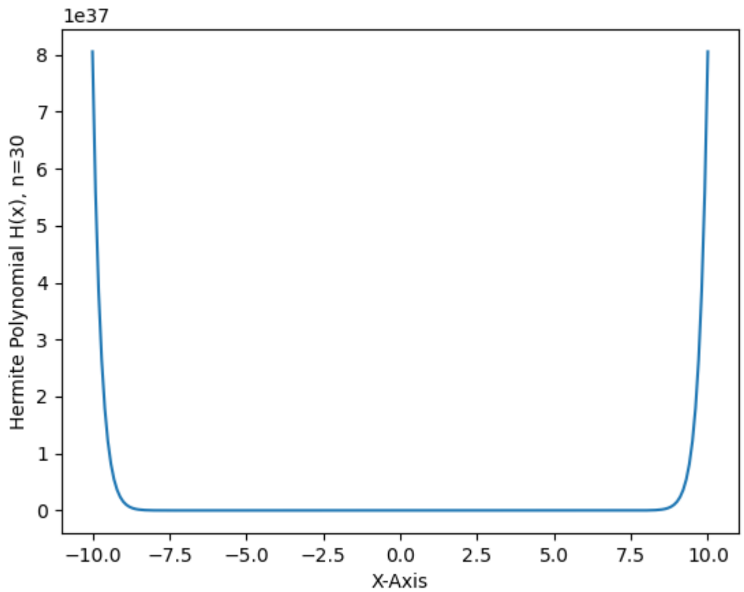

Figure 6: Hermite Polynomial $H_{30}(x)$ in the range [-10,10].

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PROBLEM 3

root mean square using Gaussian Quadrature = 2.3452078737858173
percentage error is = 2.6120914992061505e-07
root mean square using Gauss-Hermite Quadrature = 2.3452078799117153
percentage error is = 1.893602753316607e-14
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Figure 7: Comparison between Gaussian Quadrature using 100 sampling points and Gauss-Hermite Quadrature using 10 sampling points.