PHYS-GA2000-PS4

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1 Introduction

In this problem set, we are mainly interested in performing numerical integration. Specifically, we will use the so-called Gaussian Quadrature (GQ) method to solve integrals that comes up in various physical problems. Basically, what GQ does is to fit a unique polynomial expression of order $N-1$ to N data points $(x_k, f(x_k))$ where $k = 1, 2, ..., N$. It is straightforward to find the polynomial expression of order $N-1$, thus also the weights, once the non-uniformly spaced sample points x_k are specified. So, it has been demonstrated in [1] that the non-uniformly spaced sample points which correspond to integration accurate up to highest degree of freedom $2N-1$, x_k, are the zeros of the Nth Legendre polynomial.

In the first problem, we are asked to write a Python function that outputs the heat capacity of a solid as a function of temperature. We are required to use 50 sample points for GQ. And we also asked to find out how the GQ for this specific problem converges for increasing N.

In the second question, our goal is to calculate the period of an-harmonic oscillator. Harmonic oscillator is basically a particle in quadratic potential. Any other form of potential results in an-harmonic oscillatory motion which implies amplitude dependence of period. The differential equation that characterizes the dynamics of an-harmonic oscillator in 1D space is given by Eq. 1

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

where E is the total energy of the particle and V is the potential energy. We can express the dx/dt as

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

which yields

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

and if we perform the integration for the range of x from 0 to a, the amplitude, we obtain

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

Finally, if we take the constants out of the integral and make necessary cancellations, we can simplify the above equation as

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

In the third problem, we are asked to determine the $\langle x^2 \rangle$ for quantum harmonic oscillator in 1D in the 5th energy level.

2 Methods

The GQ is implemented into Python through the function **gaussxwab** written by the author of the book [1] which returns the weights, w_k, and the non-uniformly spaced sample points, x_k, for a specified number of sample points, N, and the integral limits, (a, b).

For integrals whose limits are from $-\infty$ to ∞, we need to apply change of variable. The transformation used for that purpose in this assignment is as follows

$$x = \frac{z}{1 - z^2}, \qquad dx = \frac{1 + z^2}{(1 - z^2)^2} dz \tag{6}$$

which transforms the old integration limits to -1 and 1. Using this transformation, we can appply GQ method in the same manner as before for problems in which the integration limits are from $-\infty$ to ∞.

GQ could be generalized to deal with integrals of the form

$$\int_a^b W(x) f(x) \, dx \tag{7}$$

where $W(x)$ is some function and $f(x)$ is a polynomial expression. If the dot product of two function is re-defined in the following way

$$q(x) \cdot r(x) = \int_a^b W(x) q(x) r(x) \, dx \tag{8}$$

then, it turns out that we can find complete basis set of polynomials which are orthogonal under this definition. The case where $W(x) = e^{-x^2}$ yield Gauss-Hermite polynomials. It is of great importance to notice that the integral in problem 3 can be treated this way since it involves the product of e^{-x^2} and a polynomial expression. Because of that, if we evaluate the integral in problem 3, using Gauss-Hermite polynomials, the answer should be exact.

3 Results

The results of the problem 1 are presented in Figure 1 and 2. As seen, GQ works fine even for relatively small number of sample points.

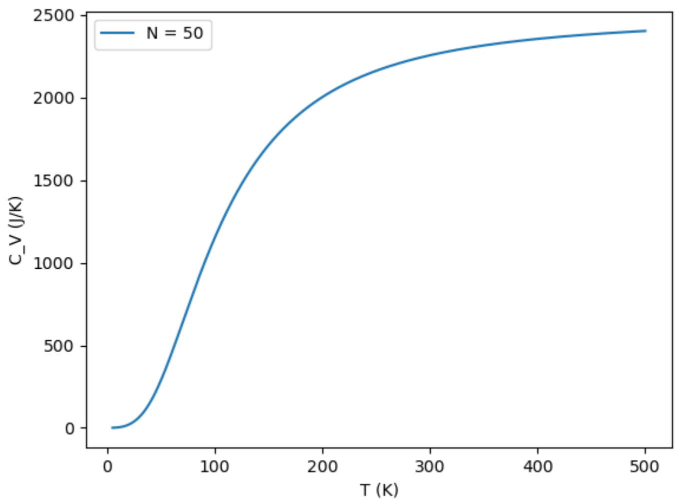

Figure 1: Heat capacity of Al as a function of T using GQ with 50 sample points.

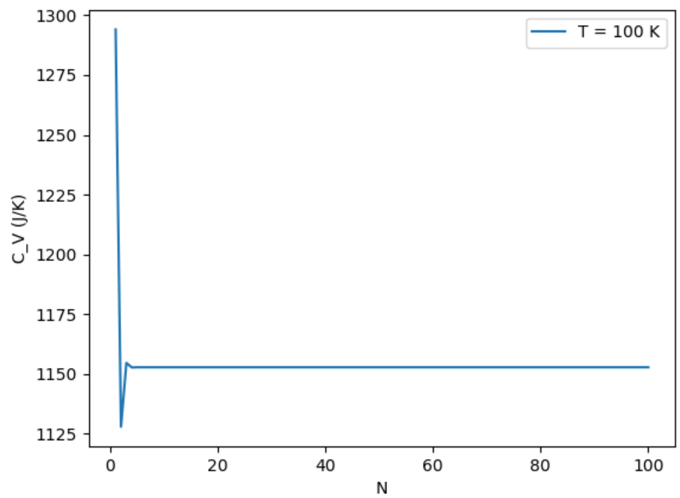

Figure 2: Heat capacity of Al at T = 100 K for different number of sample points.

The relation between the amplitude and the period of an an-harmonic oscillator is presented in Figure 3. As the amplitude goes to zero, period goes to infinity. This is because of the fact that as the amplitude goes to zero, the potential effective on the particle becomes more flat which makes it harder for particle to slide on it.

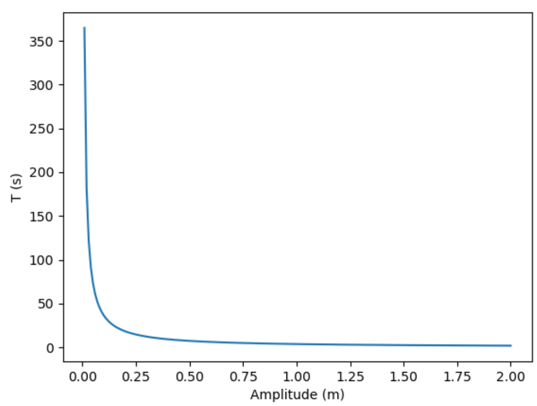

Figure 3: Period, T, of an an-harmonic oscillator as function of the amplitude, a.

The wave functions for energy levels n = 0, 1, 2, 3, 30 are presented in Figure 4 and 5. The $\sqrt{\langle x^2 \rangle}$ is calculated using Gaussian Quadrature and Gauss-Hermit Quadrature as 2.3452078737858177 and 2.3452078799117118, respectively.

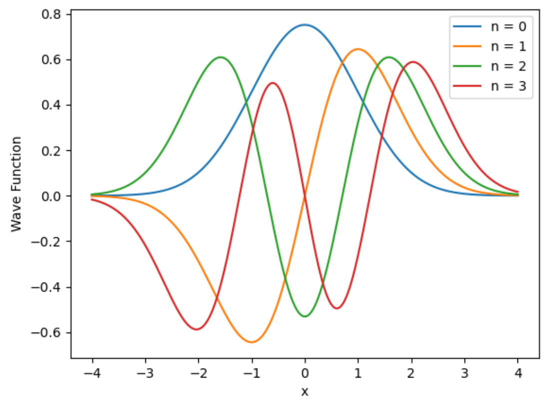

Figure 4: Wave functions of quantum harmonic oscillator for energy levels n = 0, 1, 2, 3.

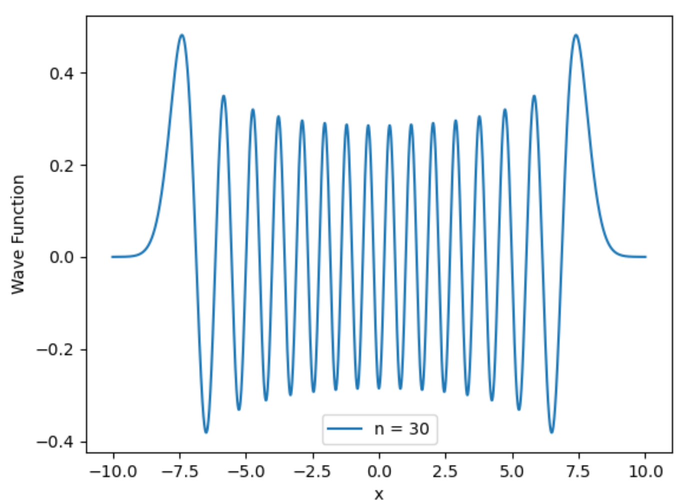

Figure 5: Wave function of quantum harmonic oscillator for energy level n = 30.

References

[1] M.E.J. Newman. *Computational Physics*. CreateSpace Independent Publishing Platform, 2013.