Computational Physics - Problem Set 4

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Github URL: https://github.com/frederikholst/phys-ga2000

1 Newman 5.9

The heat capacity of a sample of 1000 cm^3 solid aluminum with $\rho = 6.022 \times 10^{28} m^3$ and a debye temperature of $\theta_D = 428K$ is found using Gaussian quadrature integration. The weights and roots are found using numpy methods. The limits are accordingly scaled and the heat capacity is found to be 289 J/K.

The heat capacity from T=5K to T=500K is shown in Figure 1

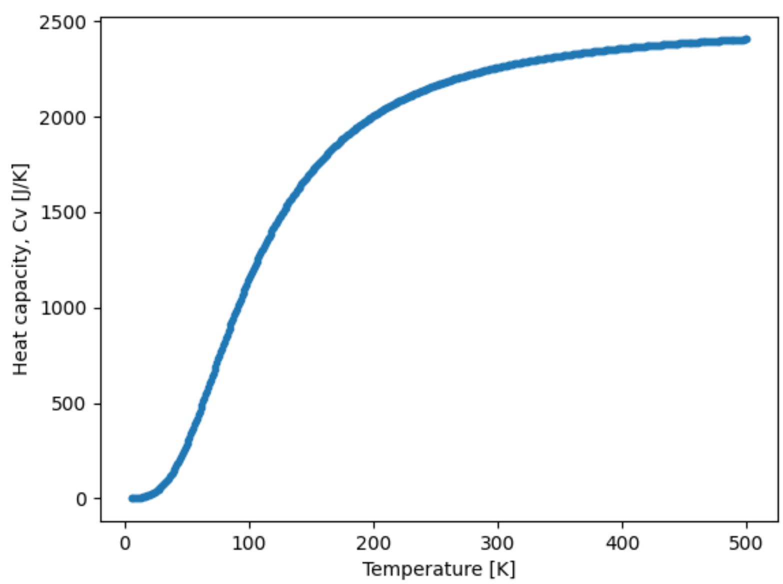

Figure 1: The heat capacity is plotted against temperature for a sample of aluminum.

Finally, Figure 2 shows how the integration converges as we increase the sample points, where we see robust results already after a very few number of sample points.

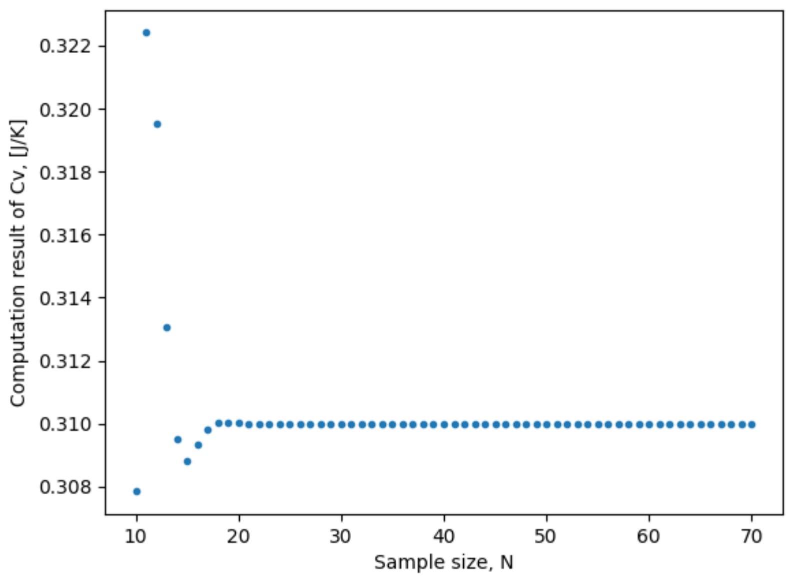

Figure 2: The computation of the heat capacity is plotted against sample points for the Guassian quadrature integration method. We see convergence already at around N=20 for T=5K.

2 Newman 5.10

We derive the period of an anharmonic oscillator, where $E = V(a)$:

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

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

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

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

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

We now set $V(x) = x^4$ and $m = 1$ and compute the period, T using Gaussian Quadratures with 20 sample points from $a = 0$ to $a = 2$ as seen in Figure 3.

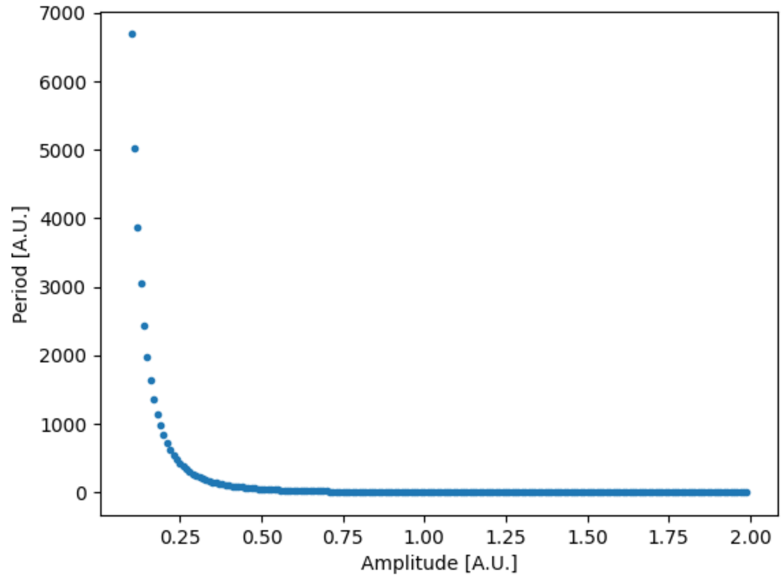

Figure 3: The period, T is computed against amplitude, a. The point a=0 is excluded to avoid dividing with zero.

We find that the oscillator swings faster and faster the larger the amplitude. This is the case for the potential, $V(x) = x^4$, because any amplitude larger than the order of unity will amplify the restoring force by a large amount. Conversely, amplitudes smaller than unity will leave the restoring force equal to zero up to third order and reduced so much with the (almost) flattened potential of x^4. In the limit of a going to zero, the motion will stop altogether, with the period going to infinity.

3 Newman 5.13

Part A: We implement a recursive function that computes the Hermite polynomials and plot the wavefunctions of the harmonic oscillator of the order n=0,1,2,3 as seen in Figure 4.

Part B: In figure 5 we see the wavefunction of order n=30:

Part C: Using first Gaussian quadrature, we compute the uncertainty of the wavefunction with 100 sample points for n=5 and achieve the result: $\sqrt{\langle x^2 \rangle} = 2.3452078799117193$.

Part D: Finally using Gauss-Hermite quadrature, we use scipy to give the roots and weights for 9 sample points and evaluate the integral to be $\sqrt{\langle x^2 \rangle} = 2.3452078799117224$. Compared to the theoretical value of $\sqrt{\frac{11}{2}}$ this gives an error of -8.43769498715119e-15. So unfortunately not exactly zero approximation error but impressively close, considering only 9 sample points.

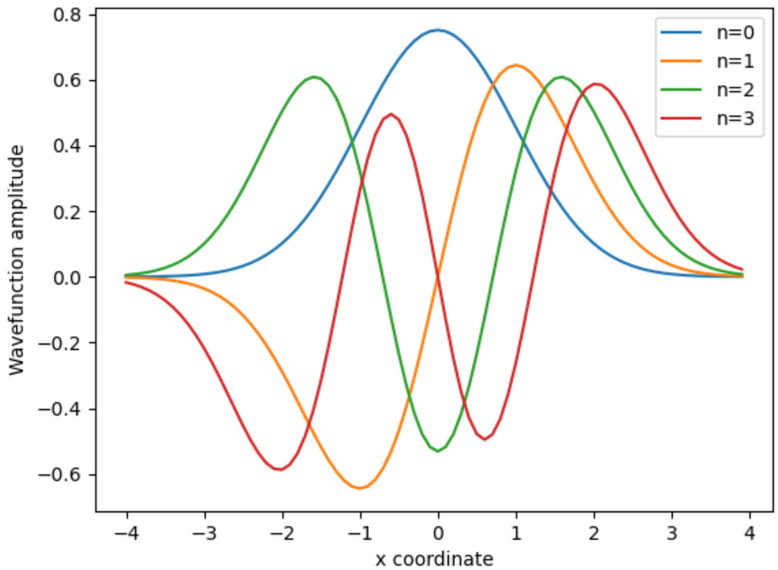

Figure 4: The four first wavefunctions of order n=0,1,2,3, are plotted in the range x=-4,x=4.

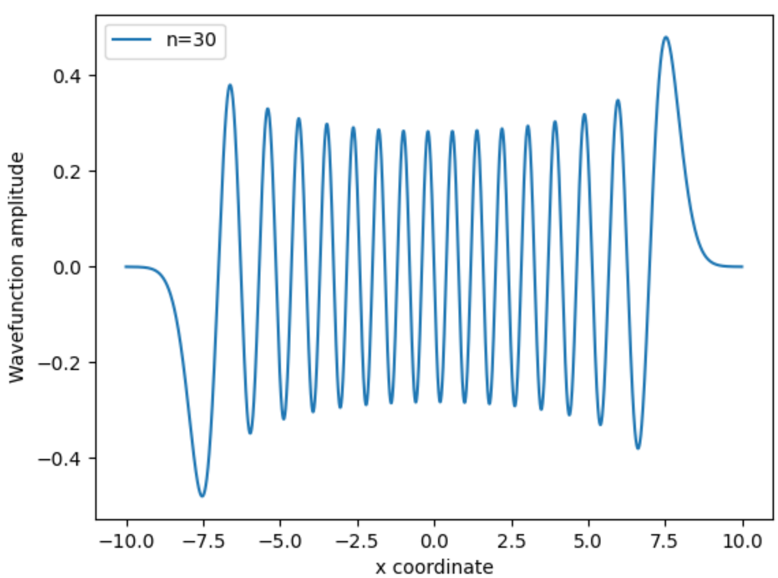

Figure 5: The wavefunctions of order n=30, is plotted in the range x=-10,x=10.