Computational Physics ps-4 Report

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1 Problem 1

1.1 Part (a) and (b)

Figure 1 shows the heat capacity as a function of temperature from $T = 5$ K to $T = 500$ K.

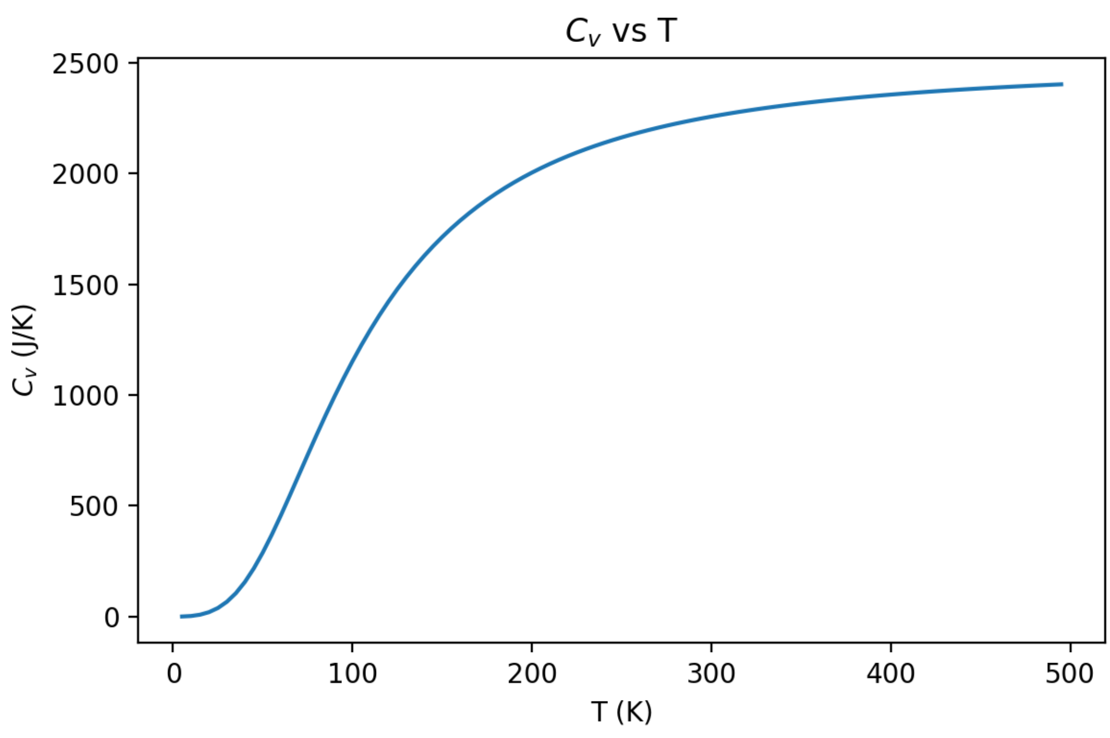

Figure 1: Heat capacity vs temperature.

According to web sources, aluminum has specific heat capacity (at 298 K) 0.90 J g^{-1} K^{-1} and density 2.7 g/cm^3. Our sample has volume 1000 cm^3. Hence its heat capacity at 298 K should be

$$0.90 \text{ Jg}^{-1}\text{K}^{-1} \times 2.7 \text{ g/cm}^3 \times 1000 \text{ cm}^3 = 2430 \text{ J/K}. \tag{1}$$

This roughly agrees with the data in Figure 1.

1.2 Part (c)

Figure 2 and 3 shows that our computation of C_v converges. Specifically, in Figure 3, where T = 5 K, we can see that C_v converges as the number of points N increases. This is reasonable as smaller T implies larger integrating interval, which may require more points to accurately compute the integral.

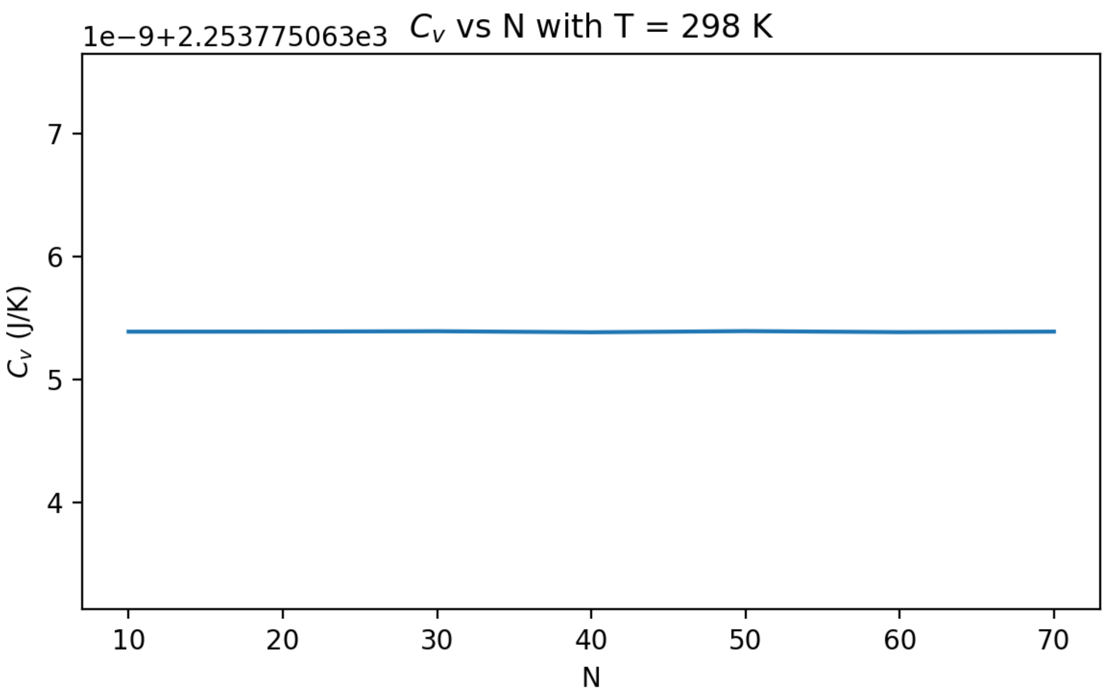

Figure 2: C_v vs N with T = 298 K.

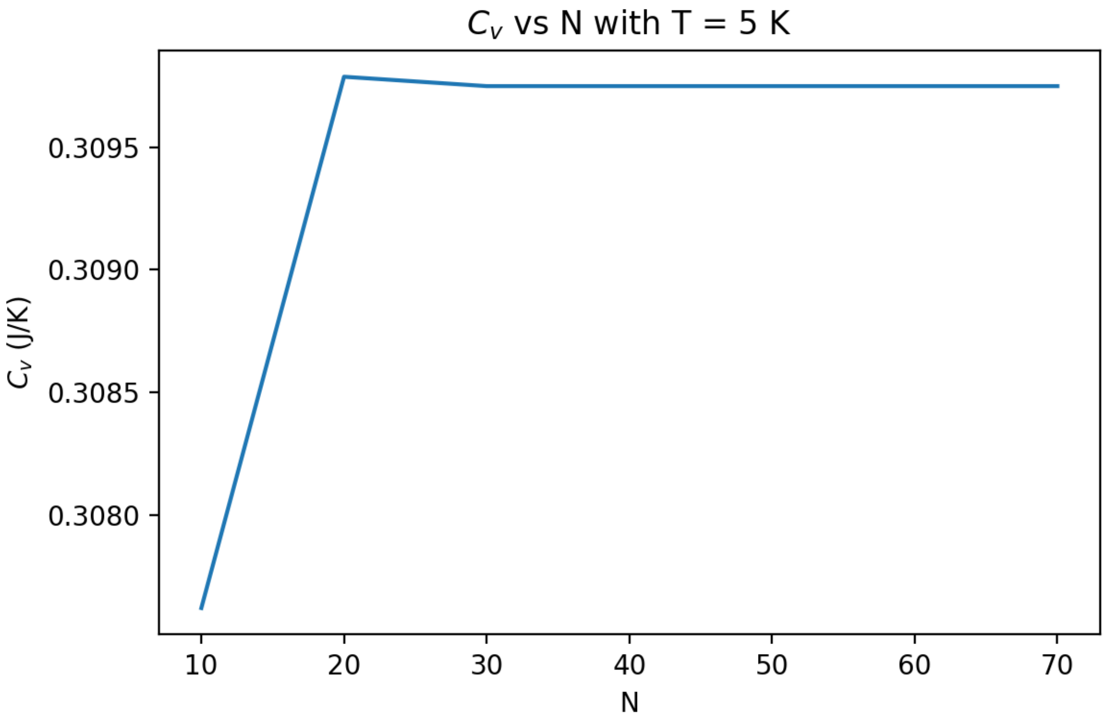

Figure 3: C_v vs N with $T = 5$ K.

2 Problem 2

2.1 Part (a)

To begin with, we have

$$\begin{cases} E = \frac{1}{2}m(\frac{dx}{dt})^2 + V(x), \\ E = V(a). \end{cases} \tag{2}$$

Rearranging, we have

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

which becomes

$$dt = \sqrt{\frac{m}{2[V(a) - V(s)]}}dx. \tag{4}$$

Integrating, we have

$$\int_0^{T/4} dt = \sqrt{\frac{m}{2}} \int_0^a \frac{dx}{\sqrt{V(a) - V(x)}}. \tag{5}$$

Finally, we get

$$T = \sqrt{8m} \int_0^a \frac{dx}{\sqrt{V(a) - V(x)}}. \tag{6}$$

2.2 Part (b)

Figure 4 shows the period for amplitudes ranging from $a = 0$ to $a = 2$.

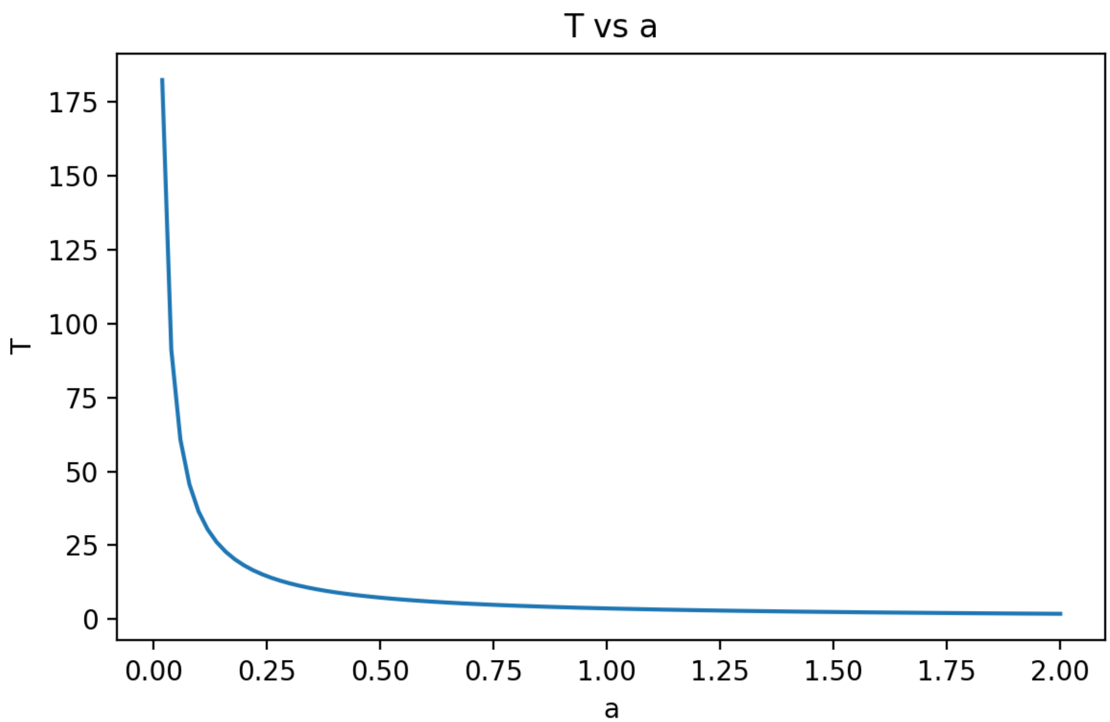

Figure 4: T vs a.

2.3 Part (c)

Figure 4 shows that the period decreases as the amplitude increases, and the period diverges as the amplitude goes to zero. This can be explained by Figure 5, which shows that

$$T \propto \frac{1}{a}. \tag{7}$$

This can also be checked by analytically finding the integral

$$\int_0^a \frac{dx}{\sqrt{a^4 - x^4}} = \frac{\sqrt{\pi}\Gamma(5/4)}{a\Gamma(3/4)}. \tag{8}$$

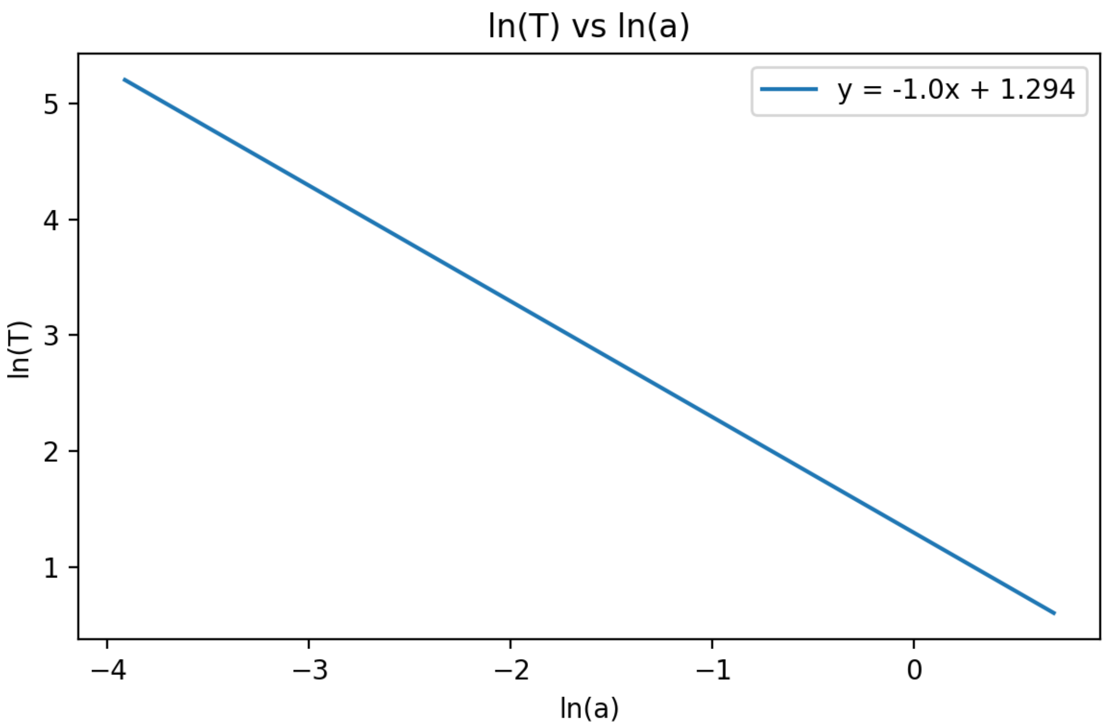

Figure 5: $\ln{(T)}$ vs $\ln{(a)}$.

3 Problem 3

3.1 Part (a) and (b)

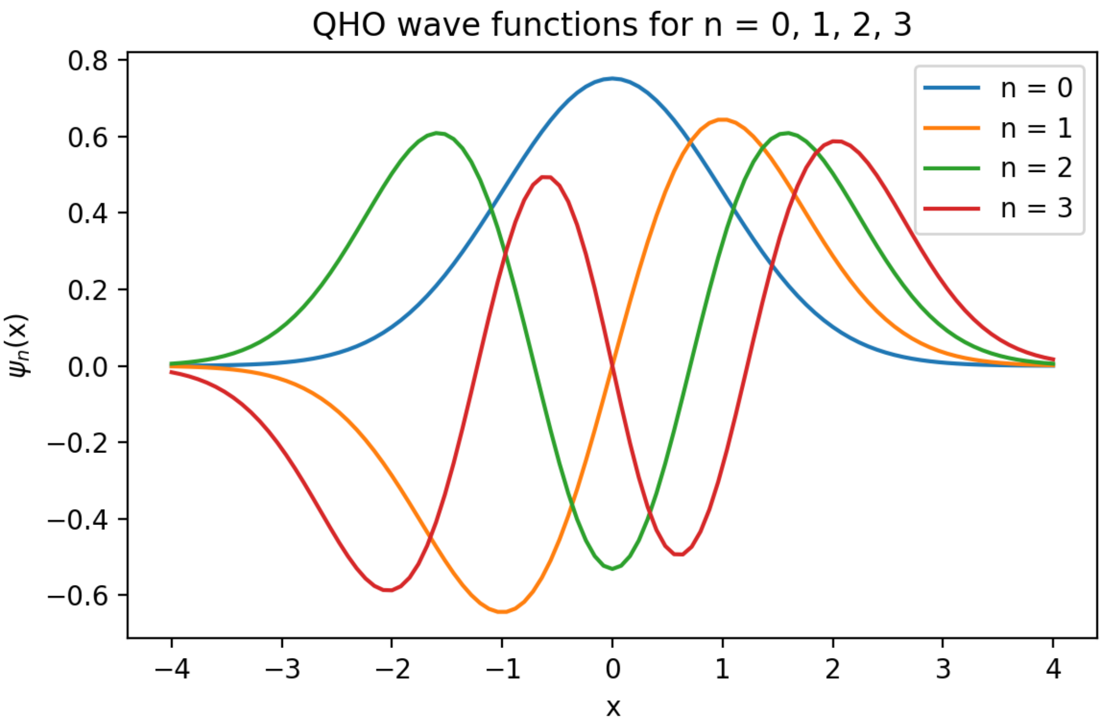

Figure 6: QHO wave functions for $n = 0, 1, 2, 3$.

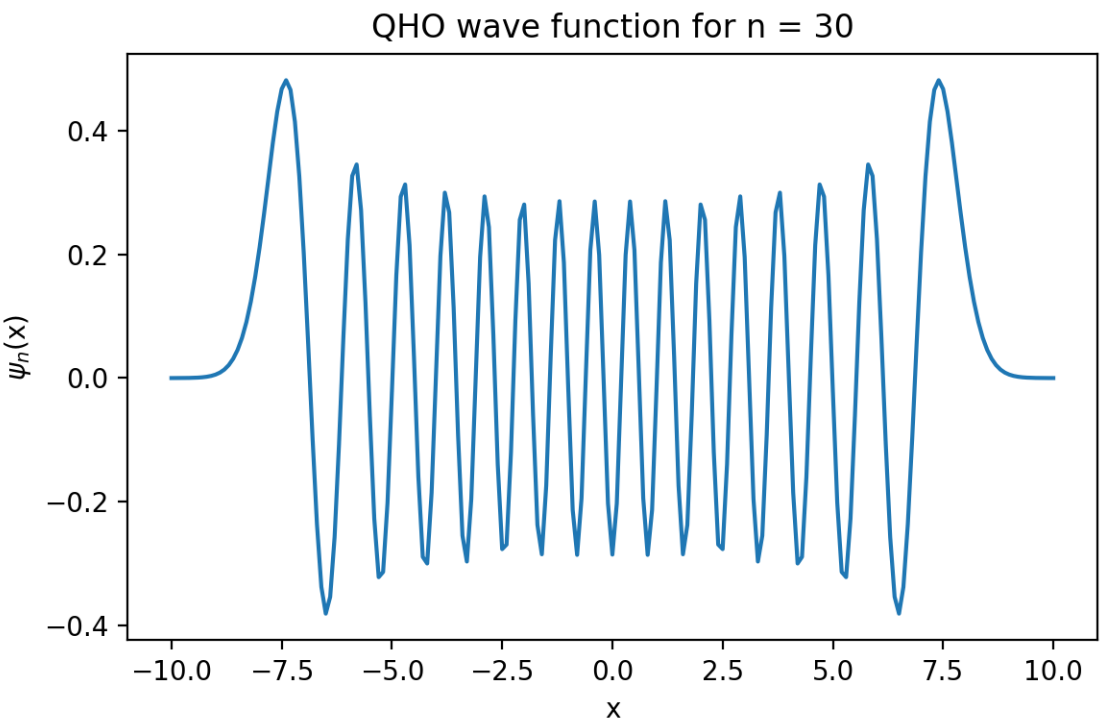

Figure 7: QHO wave functions for $n = 30$.

3.2 Part (c) and (d)

Using Gauss-Hermite quadrature, we can make an exact evaluation of the integral. Note that for $n = 5$, the polynomial in the integrand should be of degree 12, so $N = 7$ sample points should be enough for the Gauss-Hermite quadrature to give zero approximation error. We did not choose larger N here to avoid round-off errors.

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Analytical: 2.345207879911715
Gauss-Legendre quadrature (N=100): 2.3452078737858195
Gauss-Legendre difference (N=100): -6.12589534654262e-09
Gauss-Hermite quadrature (N=7): 2.345207879911715
Gauss-Hermite difference (N=7): 0.0
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