# Computational Physics: PS 4

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October 1, 2024

## 1 Discussion

My GitHub repo is `https://github.com/marcusHoskinsNYU/phys-ga2000`. For images that are blurry here, please see the ps-4 folder for individual image files.

### 1.1 Problem 1

#### 1.1.1 Part (a)

The desired Python code is given in the github repo.

#### 1.1.2 Part (b)

Using the function from part(a) above, we can plot the heat capacity as a function of temperature. Doing so in the range $T = 5\text{K}$ to $T = 500\text{K}$, we get the plot seen in figure 1.

#### 1.1.3 Part (c)

We now wish to test the convergence of our Gaussian quadrature, using several different number of sampling points. Plotting the heat capacity as a function of temperature for various $N$, we get figure 2. Zooming in around $T = 120\text{K}$, we can see the plots given in figures 3, 4, and 5. As we can see, after $N$ is greater than about 5 or 6, the plots of heat capacity seem to converge.

Alternatively, we can pick a value of $T$, let's say $T = 50\text{K}$, and plot this as a function of the various $N$. Doing so, we get figure 6, which is flat for $N > 10$, and thus implies there is good convergence of our results.

### 1.2 Problem 2

#### 1.2.1 Part (a)

We begin by saying that at time $t = 0$, our energy equation reads $E = V(a)$. Since energy must be conserved, our energy equation now reads, for general position $x$:

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

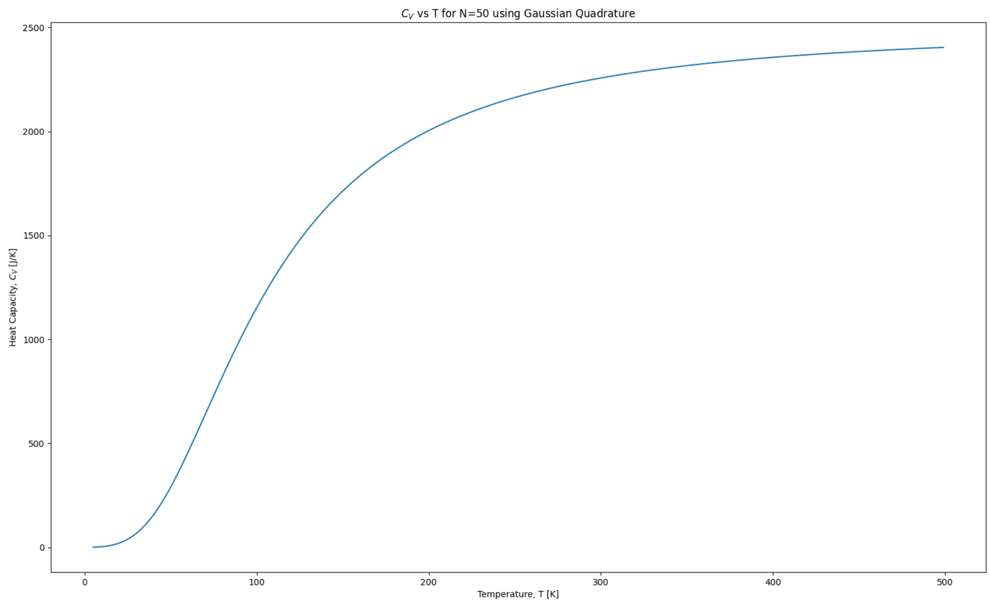


Figure 1: This is a plot of $C_V(T)$ along the range $T = 5$K to $T = 500$K, where we use Gaussian quadrature to evaluate the integral given in problem 5.9 of Newman. Here we've used 50 sample points.

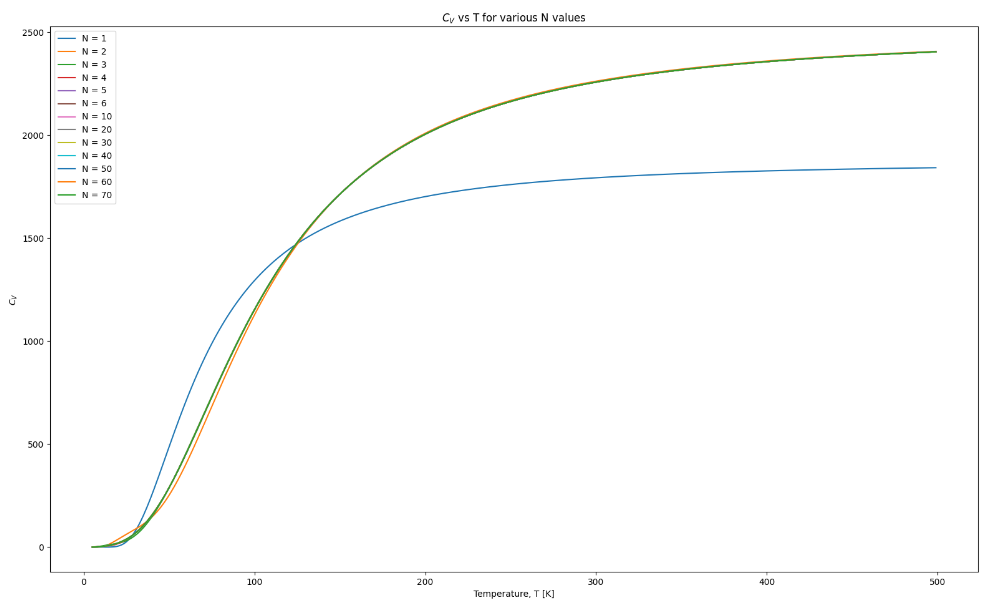


Figure 2: Heat capacity as a function of temperature for various sampling points.

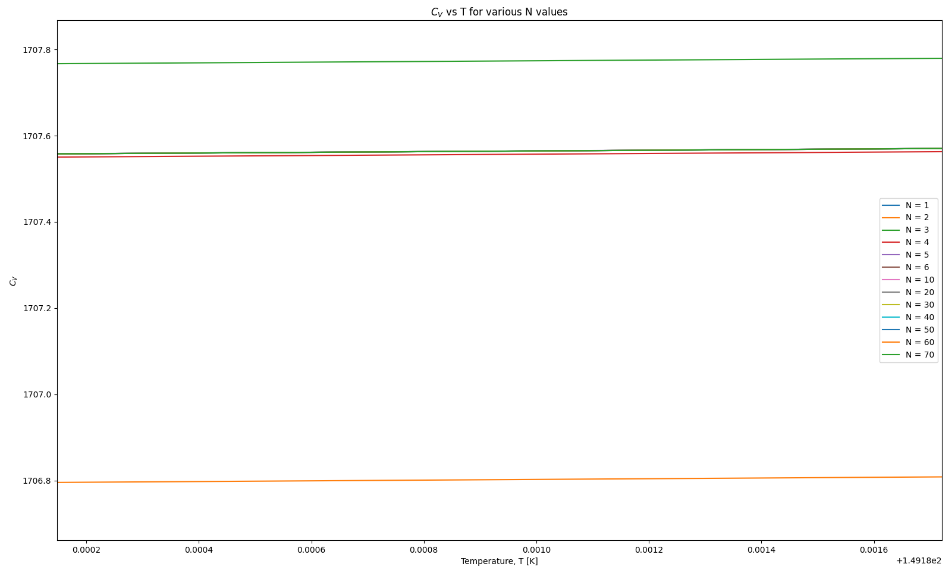


Figure 3: Figure 2 zoomed in around $T = 120$K.

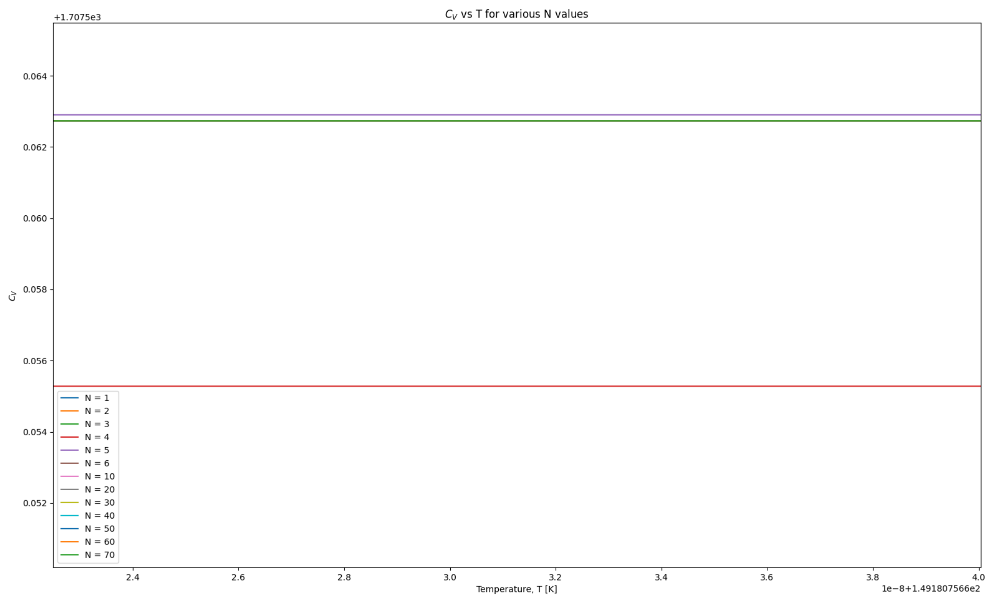


Figure 4: Figure 3 zoomed in further.

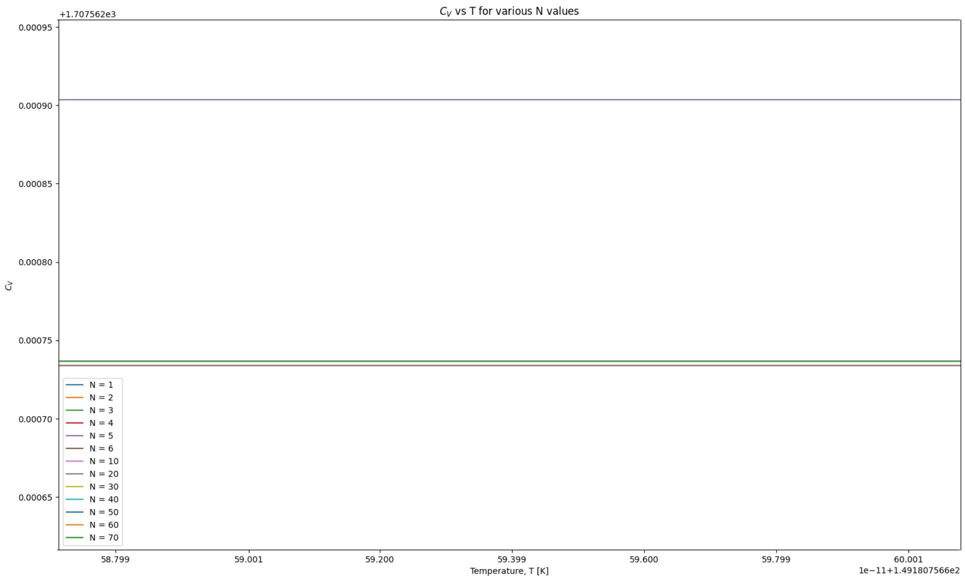


Figure 5: Figure 4 zoomed in still further.

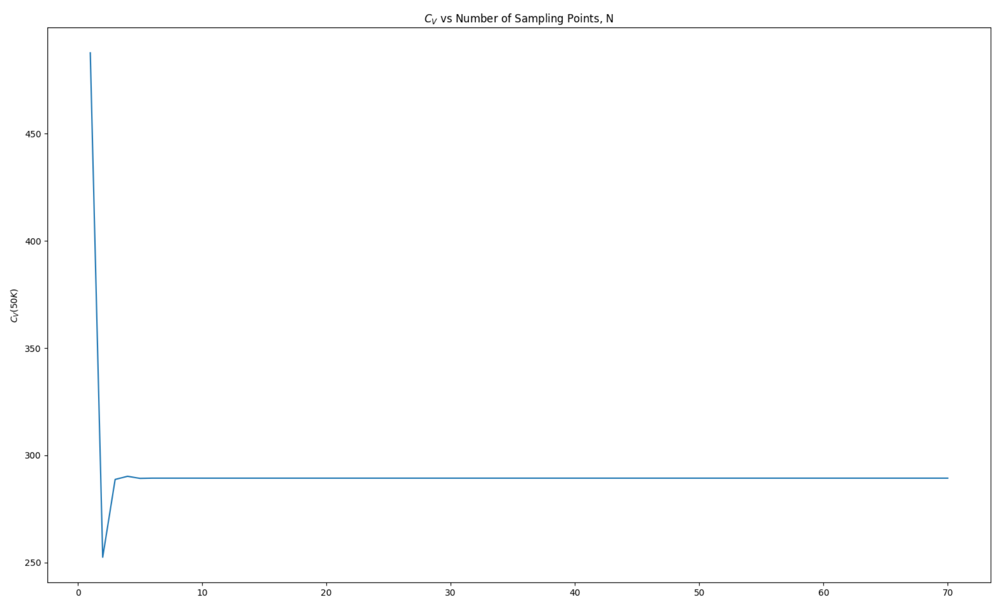


Figure 6: Heat capacity as a function of sampling point number for fixed $T = 50$K.

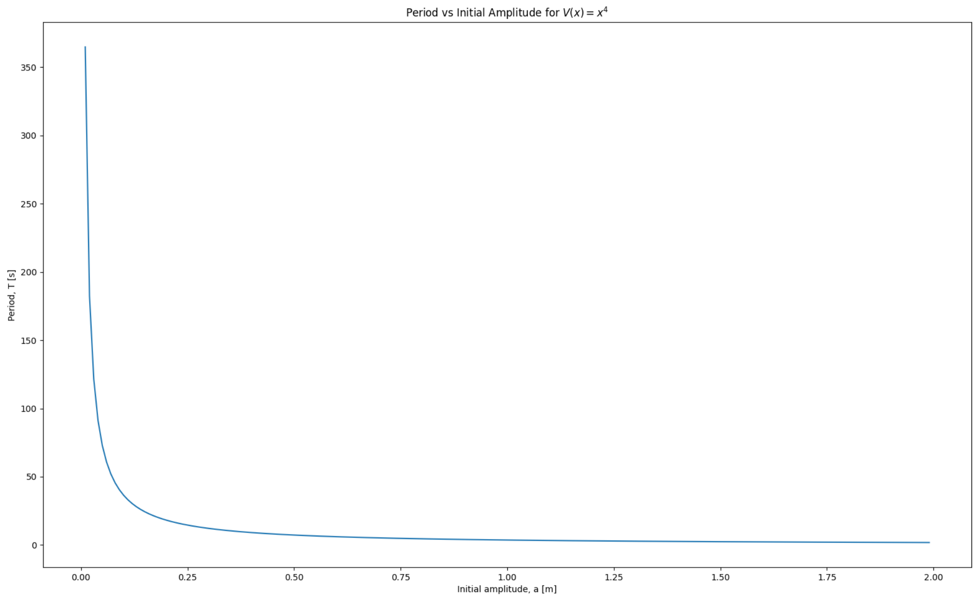


Figure 7: Period versus $a$, the initial amplitude, from $a = 0$ to $a = 2$ using the above equation. We calculate the integral using Gaussian quadrature with $N = 20$ sample points.

Then, we wish to find the period after the particle reaches $x = 0$ for the first time, or after it completes a quarter of a period. To do this, let's rearrange the above equation to read:

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

Then, integrating from $t = 0$ to $t = T/4$, or equivalently from $x = a$ to $x = 0$:

$$\int_0^{T/4} dt = \sqrt{\frac{m}{2}} \int_a^0 \frac{dx}{\sqrt{V(a) - V(x)}}.$$

Before proceeding, we note that, as given in the statement of the problem, $V(x)$ is an even function, so that we can swap the bounds of the integral on the right. Thus, we get that:

$$\frac{T}{4} = \sqrt{\frac{m}{2}} \int_0^a \frac{dx}{\sqrt{V(a) - V(x)}} \quad \Rightarrow \quad T = \sqrt{8m} \int_0^a \frac{dx}{\sqrt{V(a) - V(x)}},$$

as expected.

### 1.2.2 Part (b)

Now we suppose that $V(x) = x^4$ and $m = 1$. Building a function that calculates period using the above equation, from $a = 0$ to $a = 2$, we get a plot given in figure 7.

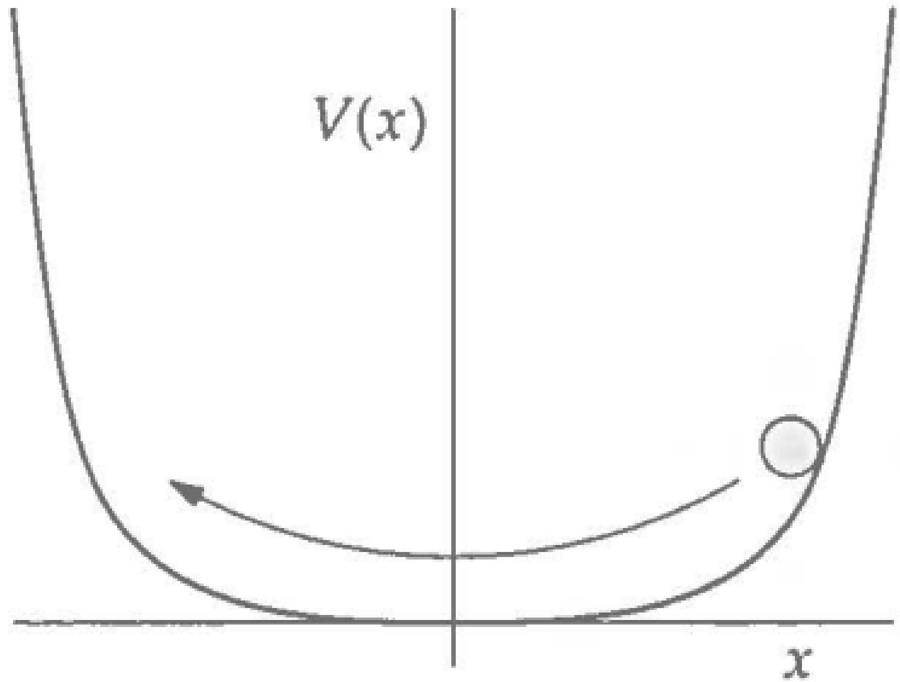


Figure 8: $V(x) = x^4$, the potential that we're considering.

### 1.2.3 Part (c)

As we see in figure 7, the period diverges as $a \to 0$, and the period decreases as $a$ increases. To explain this, we need to consider the shape of our potential, seen in figure 8. As $a$ approaches the origin, we see that our potential visually flattens out. This is also seen analytically when we look at the second derivative of $V(x)$, which tells us about the concavity. Here, $V''(x) = 12x^2$, which goes to 0 as $x \to 0$. Thus, at the origin the potential is neither concave or convex, but is flat. So, near the origin there is little effect on the particle from the potential, and so the particle does not move much at all, meaning the period is very large. On the other hand, as $a$ increases the period decreases. This is also explained by the second derivative of the potential, which increases as $x$ increases. And, as $V''(x)$ says something about the strength of the potential on the particle, we see that the particle is accelerated much more the larger $a$ is. Using a hand-wavy explanation, figure 8 gets almost vertical as we move further from the origin. Thus, it gains much more speed as it moves down the potential well.

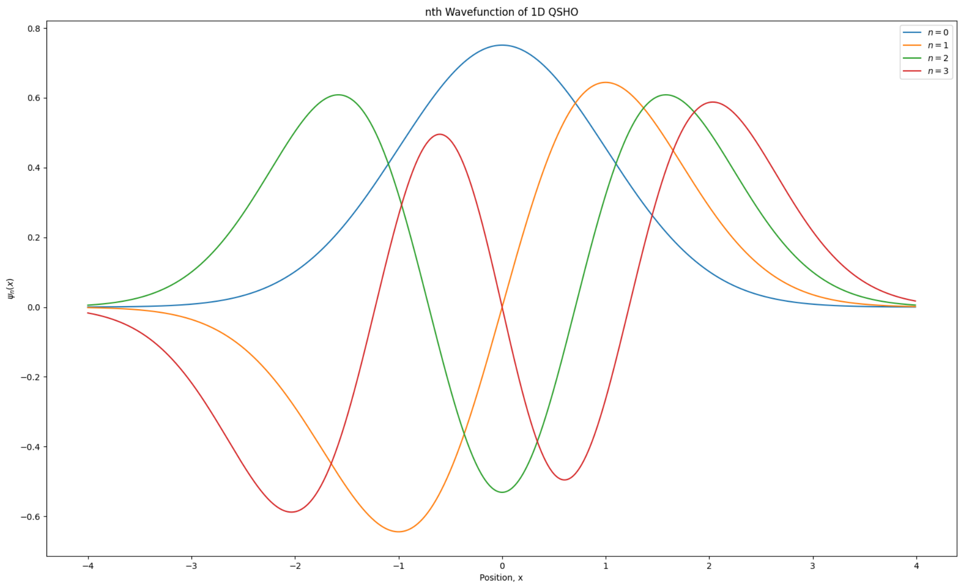


Figure 9: 1D harmonic oscillator wavefunctions for $n = 0, 1, 2, 3$.

### 1.3 Problem 3

#### 1.3.1 Part (a)

The defined function is given in the github repo, and the desired plot is given in figure 9, where the form of the wavefunction is:

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

#### 1.3.2 Part (b)

Making a plot for $n = 30$, we get figure 10.

#### 1.3.3 Part (c)

The program is in the github repo. Then, using this program, I find that $\sqrt{\mathbb{E}[x^2]} = 2.3452078799117158$.

#### 1.3.4 Part (d)

Now, using Gauss-Hermite quadrature to compute the same integral as in part (c) above, we get now that $\sqrt{\mathbb{E}[x^2]} = 2.3452078799117126$. The program for this is also in the github repo. We see the considerable agreement between these two methods.

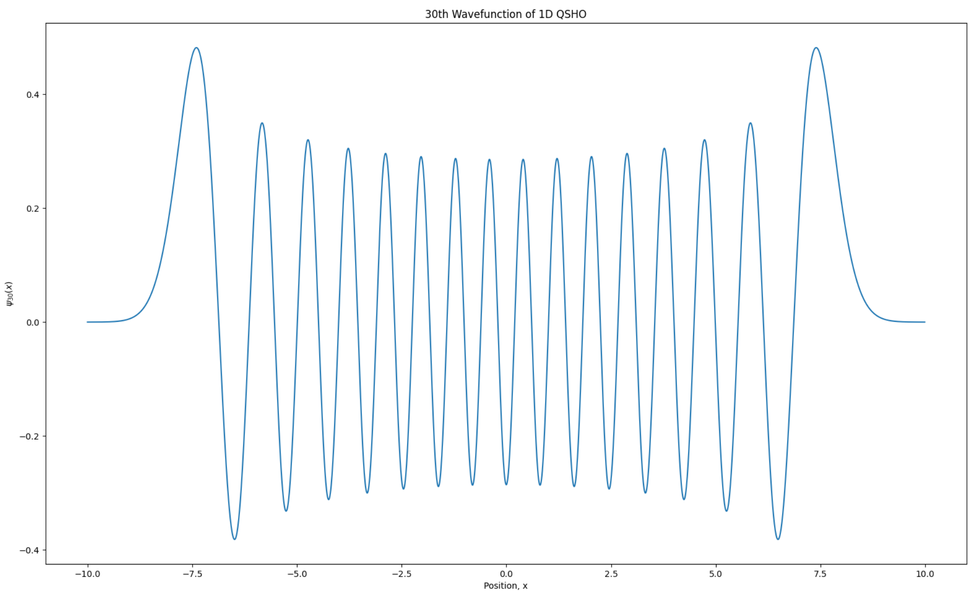


Figure 10: 1D harmonic oscillator wavefunction for $n = 30$.