Problem Set 4

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October 1, 2024

Problem 1

The heat capacity of a solid is given by

$$C_V = 9V\rho k_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \tag{1}$$

where V is the volume, ρ is the density, T is the temperature, and θ_D is the Debye temperature. I wrote a python function to compute $C_V(T)$ using Gaussian Quadrature to evaluate the integral. Figure 1 shows Cv as a function of T from 5K to 500K using $N = 10, 20, 30, 40, 50, 60, 70$. While the agreement between the different Ns appears quite good over this range, if we look at $T = 5K$ we see noticeable disagreement between the $N = 10$ value and the others (see figure 2).

Problem 2

The total energy of a particle of mass m at position x in an anharmonic potential is given by

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

where $V(x)$ in the anharmonic potential. Suppose the particle is released from rest at $t = 0$ from position $x = a$, we can replace E with $V(a)$. Rearranging the equation gives

$$dt = \frac{\sqrt{1/2m}}{\sqrt{V(a) - V(x)}} dx. \tag{3}$$

Integrating both sides over 1/4 of a period T, (x goes from 0 to a)

$$T = \sqrt{8m} \int_0^a \frac{dx}{\sqrt{V(a) - V(x)}}. \tag{4}$$

This equation can be used to determine the period of a particle with $m = 1$ in an x^4 potential. I wrote a program to compute the integral using Gaussian quadrature and to plot the period T as a function of the starting position a (see figure 3.

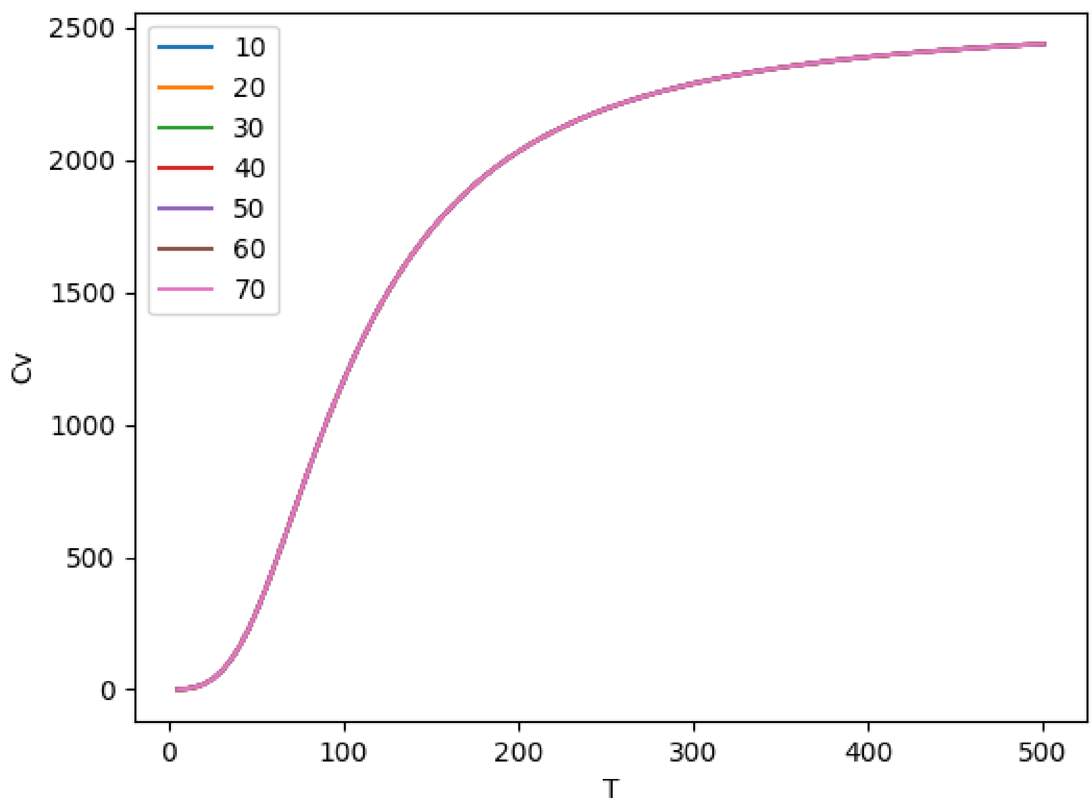

Figure 1: Plot of $Cv(T)$ at different values of N.

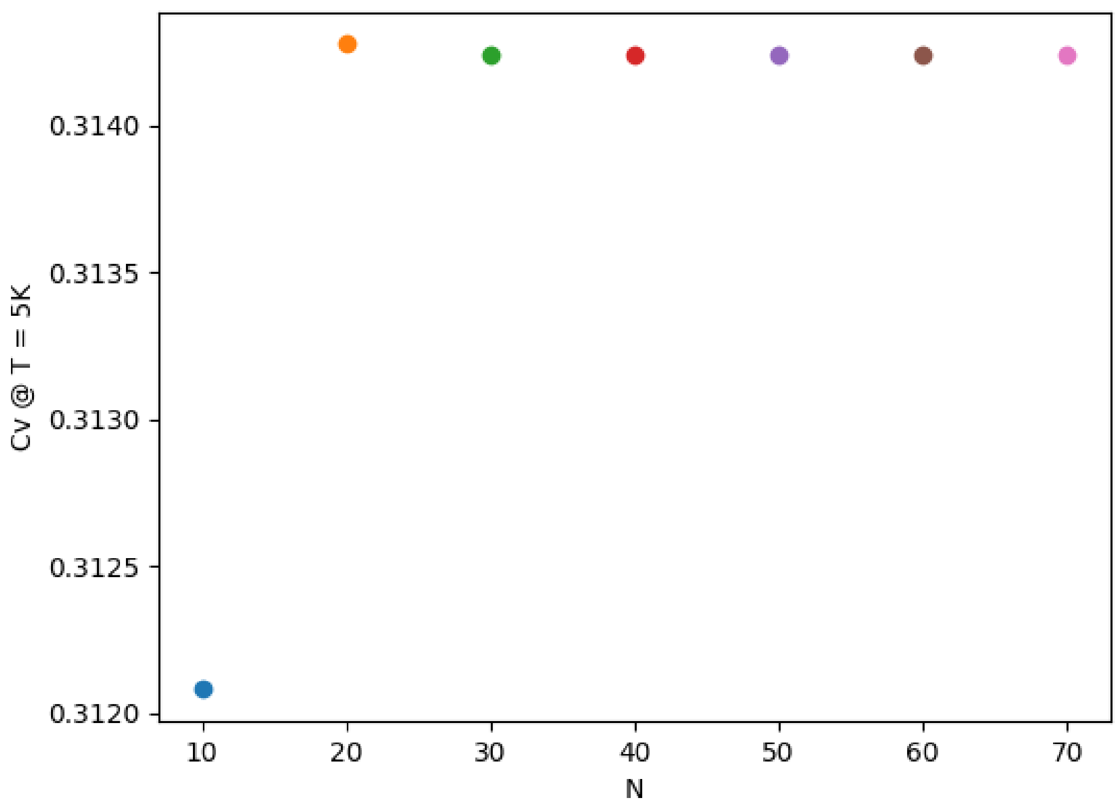

Figure 2: Plot of $Cv(5K)$ at different values of N.

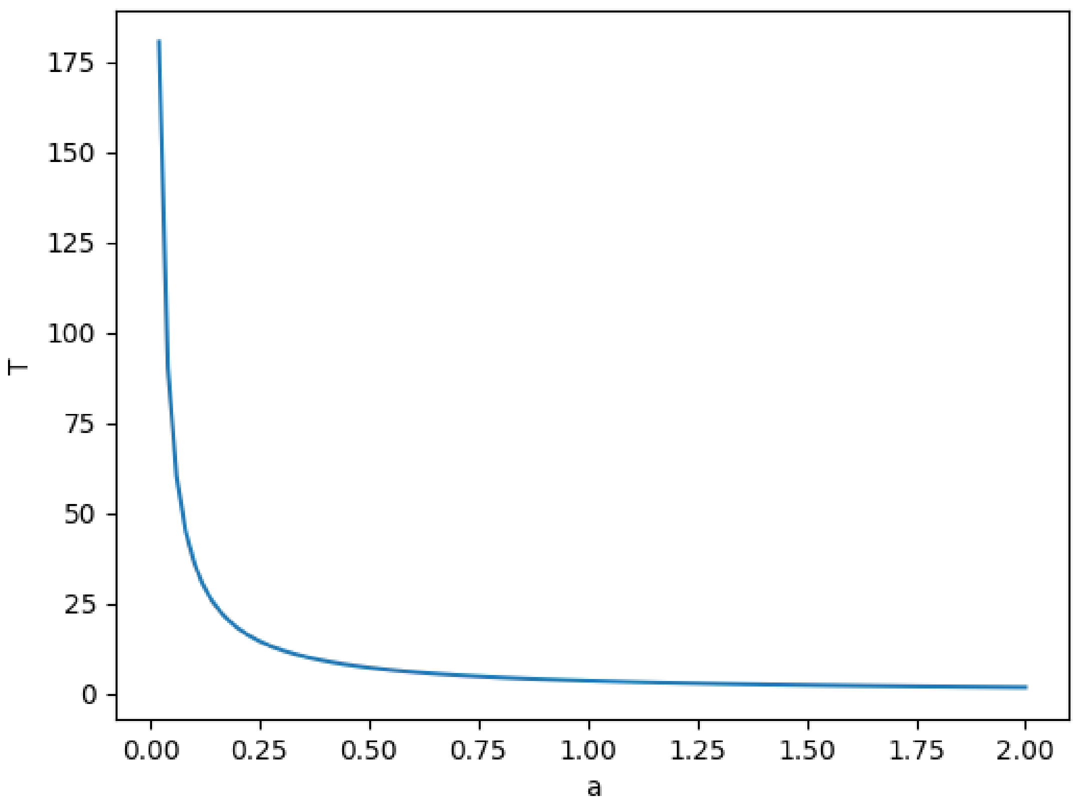

Figure 3: Plot of period T verus starting position a for an x^4 anharmonic oscillator.

The period decreases as the amplitude a increases since the velocity goes as $\sqrt{E}$ and E increases with a^4. Thus velocity goes as a^2 so increasing the position slightly increases the velocity significantly more (when $a > 1$). The period diverges to infinity as a approaches zero. This makes sense since an unmoving particle sitting at $x = 0$ can be thought of as having infinite period.

Problem 3

The wave function of spinless particle in the nth energy level of a 1D harmonic oscillator is given by

$$\psi_n(x) = \frac{1}{2^n n! \sqrt{\pi}} e^{-x^2/2} H_n(x) \tag{5}$$

where integer $n \geq 0$ and $H_n(x)$ is the nth Hermite polynomial given by the recurrence relation

$$H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x) \tag{6}$$

with the base cases $H_0(x) = 1$ and $H_1(x) = 2x$. Note that I have re-indexed the recurrence relation to give the nth polynomial rather than the $(n + 1)$th.

Part A

It is simple to implement the recurrence relation (eq. 6) with a recursive function in python. A plot of the first 4 energy levels of the harmonic oscillator was generated using such a function (see figure 4).

Part B

Figure 5 shows a plot of the $n = 30$ wave function a spinless particle in a harmonic oscillator.

Part C

The squared uncertainty in the particles position is given by

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx. \tag{7}$$

Evaluating this integral using Gaussian quadrature gives $\sqrt{\langle x^2 \rangle} = 2.345207879911708$. While this process mostly followed the process used in problems 1 and 2, a different rescaling had to be used. Since the function is symmetric about $x = 0$, we can multiply by 2 and change the limits of integration to $[0, \infty]$. This allowed me to use the rescaling function given in Professor Blanton's Juypter notebook. That function depends on a pivot point q. I used $q = 2.3$ since that is near the know average value of the function.

The integral in equation 7 can also be solved using Hermite Gaussian quadrature. This method used Hermite polynomials to find the roots instead of Legendre polynomials. Additionally, Hermite Gaussian quadrature integrates the function from $-$ to ∞ so no rescaling is needed. Also, we must

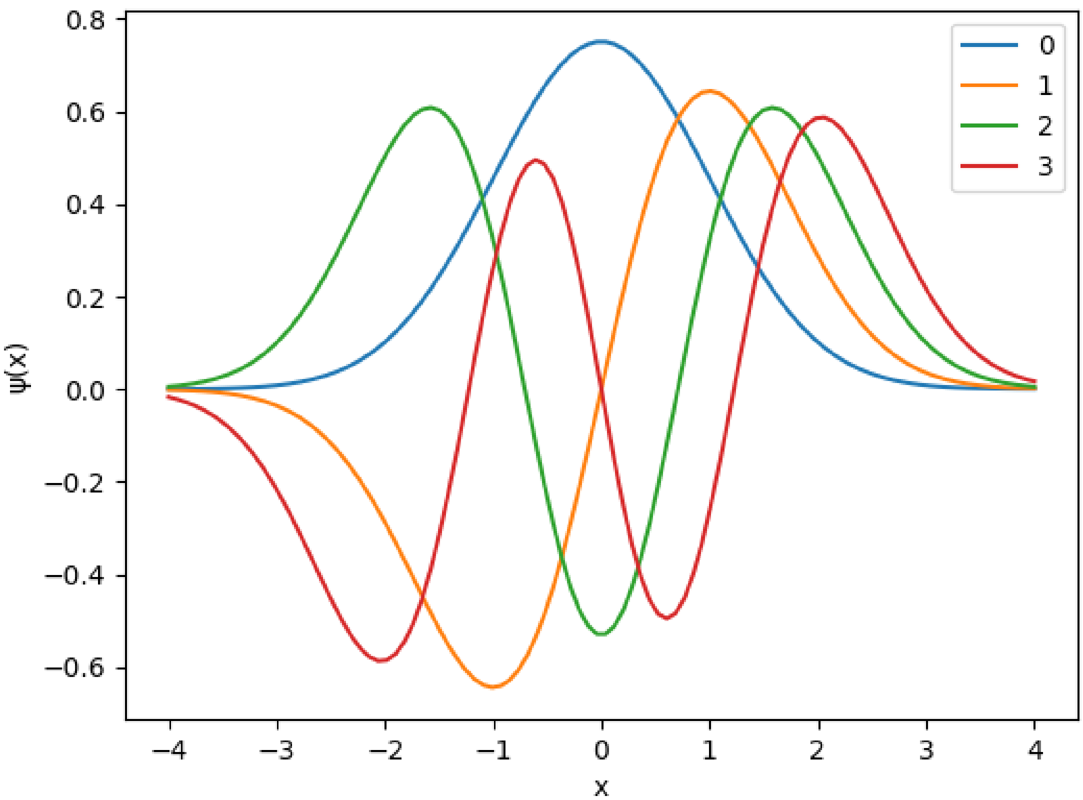

Figure 4: Plot of the $n = 0, 1, 2, 3$ wave functions for a spinless particle in a harmonic oscillator.

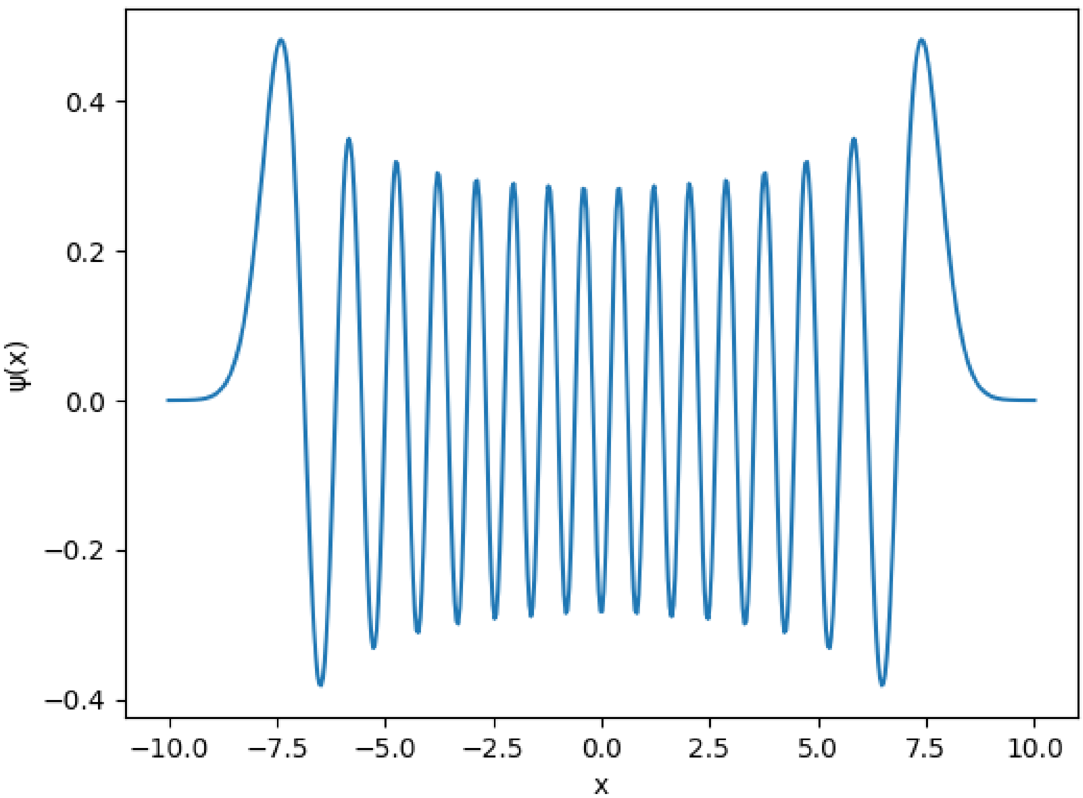

Figure 5: Plot of the $n = 30$ wave function for a spinless particle in a harmonic oscillator plotted from $x = [-10, 10]$.

multiply the integrand by a weight function e^{-x^2} which cancels out the exponential in equation 5. Using this method gave a result for $\sqrt{\langle x^2 \rangle} = 2.3452078799117144$. This should be exact (up to machine precision) since the number of points we are checking, 100, is much larger than the degree of the polynomial.