PHYS-GA 2000 Computational Physics PS4

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Prob 1:

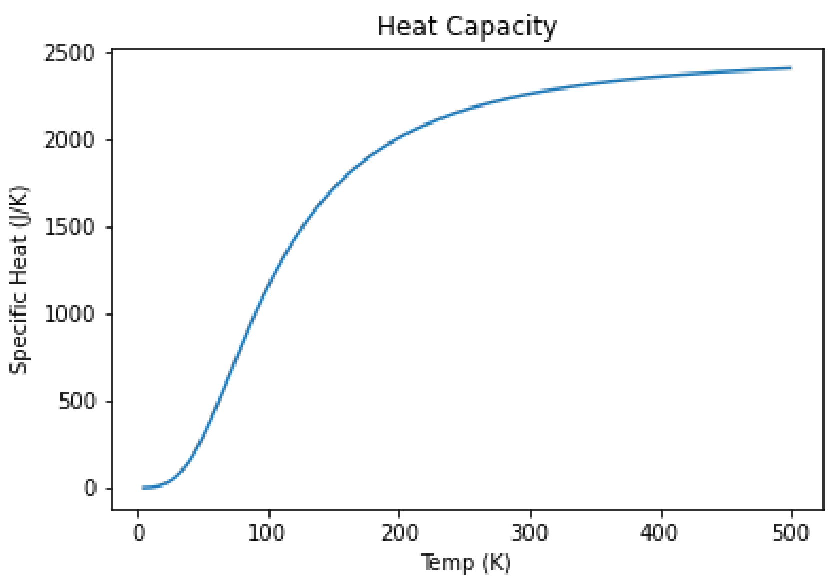

Figure 1: This figure is the heat capacity calculated with given function and constant in part a

With given function Cv, I separately calculated the coefficient $9V\rho k_b(\frac{T}{\theta_D})^3$ and the integral part $\int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x-1)^2}\,dx$. For the integral part, I adopt the method mentioned in the recitation: gaussxw returns integration points x and integration weights w. Function Cv sums up the multiplication with gaussxwab will be the Gaussian approximation of the integral.

In the convergent test, we adopt the exactly same Cv function in the first part. We evaluate the convergence at two specific temperature $T = 50K$ and $T = 200K$. We notice that the methods work well since we can tell from the

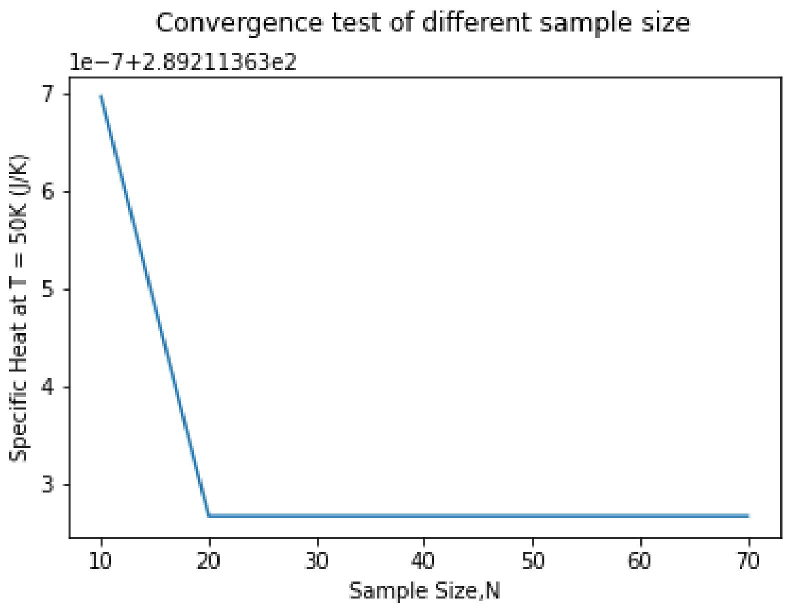

Figure 2: This figure is the Convergence test from 10 - 70 at the setting temperature 50K

figure, the y-axis index is comparatively small. We can ignore it in the actual problem working.

Prob 2:

We used two ways solving the problem.

In this problem we still use the same Gaussian approximation method, which I'll not explain again in the following part.

For the first problem with given equation, we separate the $\frac{dx}{dt}$ from the equation we get:

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

With simple integration we get the Time period equation.

For given potential $V(x) = x^4$, we redefine the integrand for given time period, $\sqrt{8m}\int_0^a \frac{1}{V(a)-V(x)}\,dx$. So we do the exactly same integration as prob 1, we get the figure.

As the potential $V(x) = x^4$, it is obvios the potential diverges faster and faster as x grows. So the conclusion in part C can be explained.

Prob 3:

With the given equation:

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

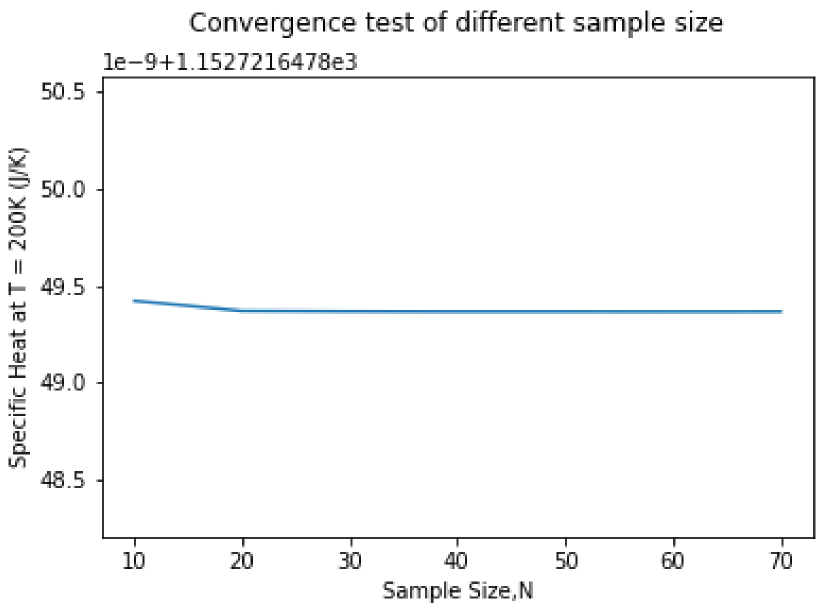

Figure 3: This figure is the Convergence test from 10 - 70 at the setting temperature 200K

We define our integration with the similar given Gaussian ways to deal with it. Notice that the $H_n(x)$ is a recursion function, which can be easily done with for loop,

In problem b, we use the function we defined in a to reproduce the result at the point $n = 30$. We still use the Gaussian quadrature here.

We adopt the Gaussian function as in the prob 1 for the part C, but we use the Hermite in the Scipy library for part D. Both of them produced the good result as we want.

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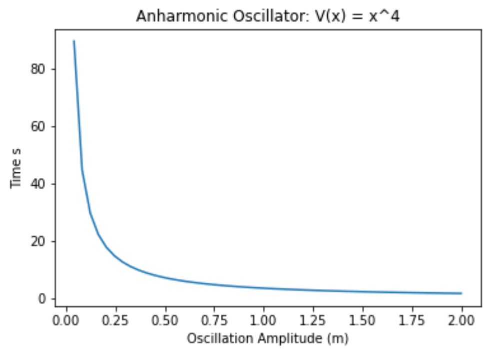

Figure 4: This figure gives the relation of the time period and the oscillation amplitude of the Anharmonic Oscillator with given potential

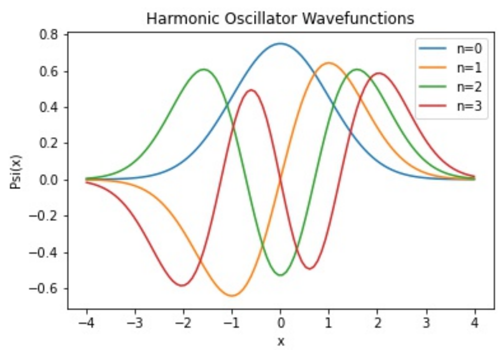

Figure 5: This figure gives the wavefunction of Harmonic Oscillator.

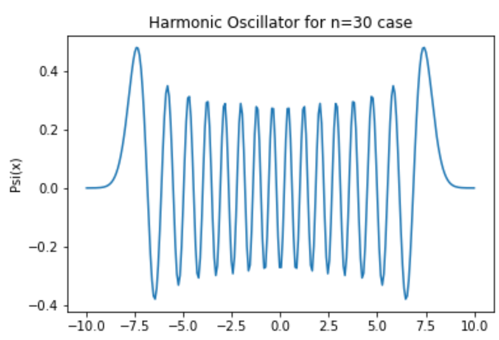

Figure 6: This figure shows wave function of Harmonic Oscillator at point n=30.

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The quantum uncertaity should be 2.3452078737858177
The quantum uncertaity should be 2.3452078799117135
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Figure 7: This result is the quantum uncertainty produced with two methods in c and d