PHYS 304 AS4

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Graded Work

1. EXERCISE 5.3 SIMPSON INTEGRAL

Given an integral,

$$E(x) = \int_0^x e^{-t^2} dt \tag{1}$$

in part(a), we are supposed to form a code that calculates the integral. For the integral part, I employ the Simpson rule.

We have,

$$I(a,b) \approx \frac{1}{3}h[f(a)+f(b)+4\sum_{oddk} f(a+kh)+2\sum_{evenk} f(a+kh)] \tag{2}$$

In the second part, we want to plot the integral value over the upper limit. I use the trick that Dan showed on Tuesday. From 0 to 1/2, I integrate over the original equation 1. For the second part, I defined a transformed version $G = \int \frac{e^{-z^2/(1-z)^2}}{(1-z)^2} dz$. Using this equation, we can make the integral toward infinity. Then, to have a more precise value, I double the N value, the number of sample points.

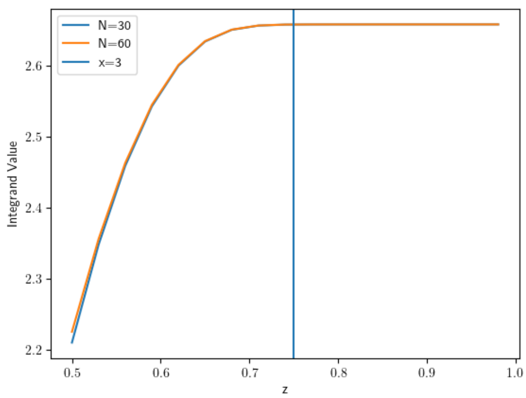

FIG. 1: [Simpson integral o er equation 1]

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In figure 1, I insert a vertical line labeled as $x = 3$, which is the upper limit set in the problem. However, in this plot, the x-axis is z, which is the variable for the transformed integral. The z value goes toward 1, which is infinity for the original function.

2. EXERCISE 5.9 HEAT CAPACITY

In Einstein's quantum model, degrees of freedom freeze out at the temperature below the oscillator frequency. The heat capacity drops like an exponential curve. The Einstein frequency is a fitting parameter [1], which is pretty accurate. However, it still fails to capture the phenomenon of some materials showing that the heat capacity is proportional to T^3. In 1912, Peter Debye found a better model and treated the quantum mechanism of the oscillation of atoms as a sound wave.

In this problem, we are given an equation of heat capacity based on Debye's theory. In part (a), I encoded a script to calculate the heat capacity given a temperature. Here, I employ the Gaussian quadrature method for the integral. First, I input the equation and collect all prefactors. I call them as CV_c. Then, I import the "gaussxw" file from the website https://public.websites.umich.edu/~mejn/cp/chapters.html. Then, I set my weight and space function by calling the "gaussxw" file. I set up two rounds of loops, one for temperature and one for sample points. The sample points loop sits inside the temperature loop. One crucial lesson from Dan's help hour is that the integral needs to be set equal to zero every time before the sample points loop, so that the new integral starts from zero instead of adding to the previous value.

In Figure 2, I use the Simpson method to do the calculation, while in Figure 3, I use the Gaussian Quadrature method. As we can tell, when the temperature is high enough, the heat capacity tends to flatten out, around 10^5. This is slightly high than expected in Debye's model. Since it's approximate, it's close enough. One way to examine the integral is to take the extreme values. When the temperature approaches zero Kelvin, the integral part is around 1; then, the prefactor dominates the heat capacity value, which should be a cubic proportionality. When the temperature approaches infinity, the temperature dependence is canceled out, and a flat line is shown on both plots.

Survey Questions

I took 5 hours for this week's homework. I learned an important lesson from Gaussian Quadrature. Make sure

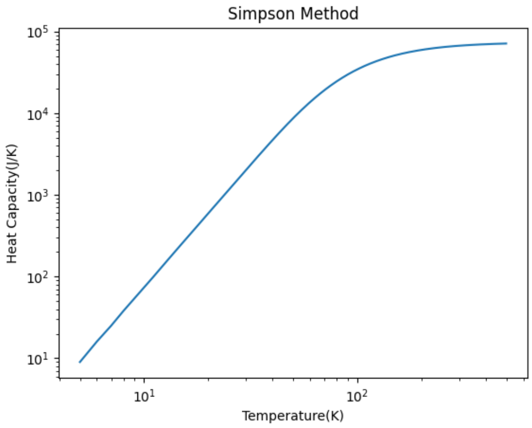

FIG. 2: [Heat capacity problem using Simpson method]

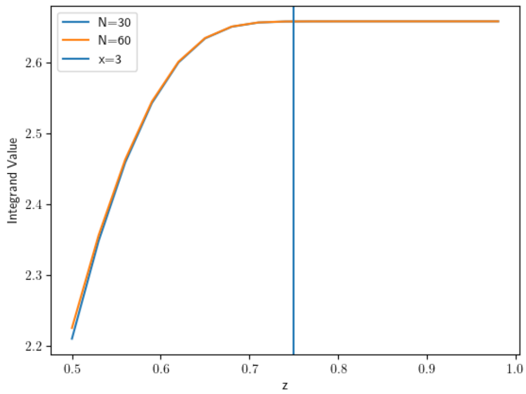

FIG. 3: [Heat capacity problem using Gaussian Quadrature method]

the integral equals zero every time before starting a new one (like a new loop of a new calculation). I like the heat capacity problem most! I think this problem set is about the right length.

Ungraded Work

I have downloaded the repository.

I have followed the class notes and understood every step.

I have completed the tutorial posted on Moodle.

[1] S. H. Simon, *The Oxford solid state basics* (Oxford University Press Oxford, Oxford, 2016), first edition, reprinted (with corrections) ed., ISBN 978-0-19-968076-4 0-19-968076-0 978-0-19-968077-1 0-19-968077-9, section: xv, 291 Seiten : Illustrationen, Diagramme.