# Hw 4

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[Learned the computation of the error function through integral of a Gaussian and evaluate the heat capacity of a solid using Trapezoidal integration ]

## 1. INTRODUCTION

For this homework assignment, we learned a few ways to evaluate integrals. One of this ways in to use the Trapezoidal rule, which approximates he area as a set of trapezoids, and is usually more accurate. In other words, it gives us a trapezoidal approximation to the area under one slice of the function, given by this equation:

$$A_{\mathrm{k}} = 1/2h[f(a+(k-1)h) + f(a+kh)] \tag{1}$$

To get this, suppose we divide the interval from $a$ to $b$ into $N$ slices, so that each slice has the width $h = (b-a)/N$. Then, the right-hand side of the kth slice falls at $a+kh$, and the left-hand side falls at $a+kh = a+(k-1)h$ resulting in Equation 1.

Now, to get the approximation for the area under the whole curve is the sum of the areas of the trapezoids for all $N$ slices:

I(a,b) $\approx \sum_{k=1}^{N} A_{\mathrm{k}} = \frac{1}{2}\sum_{k=1}^{N}[f(a+(k-1)h)+f(a+kh)]$
$= h[\frac{1}{2}f(a) + f(a+h) + f(a+2h) + .... + \frac{1}{2}f(b)]$
$= h[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)]$. (2)

For this formula, the quantity inside of the brackets is a sum over the values of $f(x)$ measured at equally spaced points in the integration domain and we take a half of the values at the start and end points but one times the value at all the interior points.

Another technique for evaluating integrals is using the Simpson's rule, which obtains a more accurate result by using quadratic curves while still getting an answer quickly. Using this method, we approximate the integrand with quadratics by taking a pair of adjacent slices and fit a quadratic through three points that mark the boundaries of those slices, then we calculate the area under those quadratics which gives an approximate to the area under the curve.

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## 2. EXERCISE 5.3

For this exercise, using the integral:

$$E(x) = \int_0^x e^{-t^2}\, dt \tag{3}$$

I had to write a program to calculate $E(x)$ for values of x from 0 to 3 in steps of 01, and then make a graph of $E(x)$ as a function of x. To calculate the integral, I choose to use the trapezoidal rule, and started by defining the function to integrate ($e^{-t^2}$). I then defined the trapezoidal integration with three arguments (a, b , N) and added a loop to compute the sum of the trapezoidal areas under the curve of f(t) at each step i, and add up the results to obtain the value of the integral E(x). I chose N to be 30 because I thought it was a reasonable accuracy without compromising the efficiency. I then proceeded to calculate $E(x)$ for values of x from 0 to 3 in steps of 0.1. Finally I created the x and y values lists, so that I could plot the graph.

## 3. EXERCISE 5.9

For this exercise, I was given Debye's theory of solids that gives the heat capacity of a solid at temperature T to be:

$$C_{\mathrm{V}} = 9V\rho k_{\mathrm{B}}(\frac{T}{\theta_{\mathrm{D}}})^3 \int_0^{\theta_{\mathrm{D}}} \frac{x^4 e^x}{(e^x-1)^2}\, dx \tag{4}$$

where $V$ is the volume of the solid, $\rho$ is the number density of atoms, $k_{\mathrm{B}}$ is Boltzmann's constant, and $\theta_{\mathrm{D}}$ is the so called $Debyettemperature$, a property of solids that depends on their density and speed of sound. To write a program a function cv(T) that calculates Cv for a given value of the temperature, for a sample consisting of 1000 cubic meters of solid aluminum, which has a number density $\rho = 6.022x10^{28}m^3$ and a Debye temperature of $\theta_{\mathrm{D}} = 428K$.

To create this program, I started by defining the integral given in the end half of the equation. I then define the function to calculate $C_{\mathrm{V}}$, which included me defining the constants given in the problem as well as the integration limits. I then also used the trapezoidal rule to do the integration and added a loop to compute the sum of the trapezoidal areas under the curve of f(x) at each step i. Finally, to calculate $C_{\mathrm{V}}$ I input the complete formula including the integral evaluated using the trapezoid rule. Same as in the previous exercise, to create a graph of the heat capacity as a function of temperature from $T = 5K$ to $T = 500K$, I created a lists containing temperature and $C_\mathrm{V}$ values, and plot them.

## 4. RESULTS

For exercise 5.3, I got the following graph:

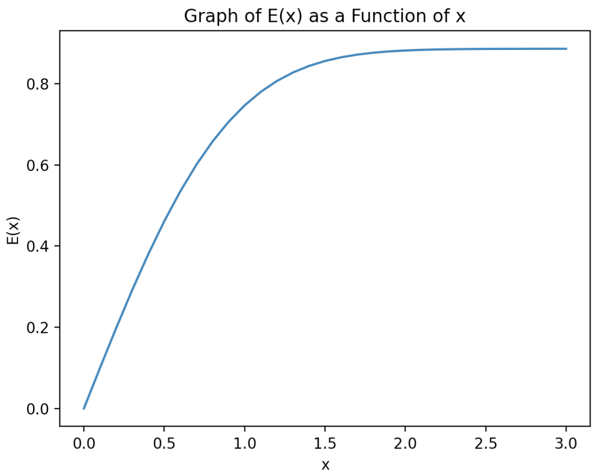


FIG. 1: $E(x)$ as a function of x for x values from 0 to 3 in steps of 0.1

For exercise 5.9, I got this graph showing the heat capacity as a function of temperature.

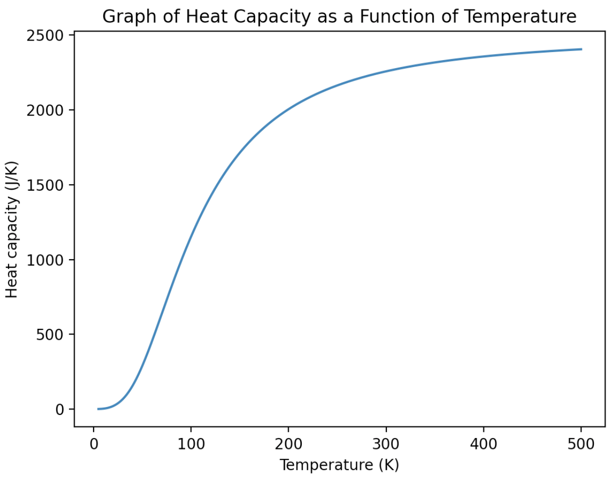


FIG. 2: Graph showing the heat capacity as a function of temperature from T =5K to T= 500K

## 5. CONCLUSION

Survey Questions For this assignment, it took me a long time mainly because I had so much trouble trying to write the program for 5.9. For some reason I kept getting a zero division error: float division by zero. Which is when I asked Emma for advice, and she told me that maybe an if statement would help, which it did!. I feel like I ;earned a lot on this assignment, and not only in the physics part but I am definitely getting more comfortable with LATEX! mainly with imputing commands, like a couple of assignments before I didn't know how to add the limits to the integral but now I know, and I think that my typing speed is improving a lot. Both problems were kinda similar, so both were interesting to me, and I got to try making a flow chart since I still don't know which I prefer between the chart and pseudo code. .