

# PHYS H304 Homework 4

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This is the lab report write-up of the approach and methods used for the fourth problem set in PHYS H304.

## 1. INTRODUCTION

This is a summary of the methods and major equations used for this problem set. In this report, we explore methods of numerical integration, focusing largely on the application of Simpson's rule and errors on approximations of integration methods. We present the plots we produced representing the evaluation of integrals of various functions and error on the integral approximation for various widths and slices used in the approximation. The major equations used are included where appropriate and a summary of the approach used to develop the code is included as well. All equations are taken from Computational Physics by Mark Newman [1].

## 2. METHODS

### 2.1. Exercise 3.6

For Exercise 3.1, we are asked to estimate the integral of the function given in Eqn. 1. Of the two integration methods covered before exercise, Newman [1] proves that Simpson's rule yields a more accurate value. To evaluate Simpson's rule, we use Equation 5.10 from [1], reproduced in our Eqn. [? ].

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

$$I(a, b) \cong \frac{h}{3} [f(a) + f(b) + 4 \sum_1^{N/2} f(a + (2k-1)h) + 2 \sum_1^{N/2-1} f(a + 2kh)] \quad (2)$$

Hence, Simpson's rule operates by approximating an integral by summing the weighted values of a given function over "h" number of slices. These weights are determined by the nature of Simpson's rule that operates by approximate the area under an appropriate number of quadratic functions fitted to the curve. To do so, it slices the area under the curve into sections such that each pair of sections is used to estimate the area under a quadratic curve. When summing over these contributions, the sections representing an even multiple of slices from the lower limit of the integral appears twice in the sum due to the dependence of the coefficients on the number of slices. Similarly, the sections representing

an odd multiple of slices appear four times in the sum of the function over the range of integration.

To evaluate the sum, Simpson's rule dictates that the approximation is given by the sum of the function evaluated at the upper and lower limits of the integral and the values of the function evaluated at the odd and even multiples of the slices scaled by four and two respectively. We code Eqn. 2 in Python defining a function that outputs the values of the integral after computing the sum of each of the odd and even contributions over the range of slices.

For this exercise, we determined a suitable number of slices by requiring a precision of  $10^{-3}$  in our approximation. To determine the corresponding number of slices, N, to this precision, we made a logarithmic scale plot of the error on the integral approximation using Simpson's rule of Eq. 1 at a fixed value of  $x=2$  for a range of N from 1-100. The error was determined by using the recursive method discussed in the lecture notes shown in Eq. 3 where  $E(x)_{currentN}$  is the approximation of the integral for a given number of slices and  $E(x)_{priorN}$  is the approximation for the previous attempt of the number of slices.

$$E = \frac{E(x)_{currentN} - E(x)_{priorN}}{E(x)_{currentN}} \quad (3)$$

We estimated the approximate value of N that resulted in a  $10^{-3}$  precision by reading the value from the plot we made of the error for different values of N. Then, we determined the width of each slice by using Eqn. 4 using the lower limit  $a = 0$  and allowing the upper limit, x, to range from 0-3.

$$h = \frac{x - a}{N} \quad (4)$$

Substituting the values of h and N into Eqn. 2, we determined the integral of the exponential function for values of x ranging from 0 to 3. We then produced a plot of the approximations of the integral against this range of x values.

### 2.2. Exercise 3.8

Molecules are generally formed by atoms bound by specific energies. Debye models the oscillations of atoms in the solid state as that of phonons. [2] As thermal energy is proportional to temperature, so is the heat capacity,

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which corresponds to units of thermal energy per unit temperature (J/K). An estimation of the heat capacity based on Debye's theory is given in [1] [2] shown in Eqn. 5

To evaluate the integral, we implement our method of applying Simpson's Rule described in ???. Since, we are told  $N=50$ , we divide the sample into 50 slices of width determined by Eqn. 4. Multiplying the integral by the appropriate pre-factor, we defined a Python function that determined the value of the heat capacity for a given temperature. For the ranges of temperature between 5-500K, we plotted the approximated value of the integral as a function of temperature.

$$E_x = 9Vk_B \left( \frac{T}{\theta_D} \right)^3 \cdot \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \quad (5)$$

Observing the behavior of the integrand at the boundary limits of integration, we note that as  $x$  approaches zero, the denominator approaches zero, which would cause an error in the code. Hence, multiplying the expression to be integrated by a factor of  $\frac{e^{-x}}{e^{-x}}$ , we re-write the expression in Eq. 8.

$$\frac{x^4 e^x}{(e^x - 1)^2} * \frac{e^{-x}}{e^{-x}} = \frac{x^4}{e^x - 2 + e^{-x}} \quad (6)$$

Taking the derivative of this expression, we obtain the expression in Eqn. ???.

$$\frac{d}{dx} \frac{x^4}{e^x - 2 + e^{-x}} = \frac{4x^3}{e^x - e^{-x}} \quad (7)$$

Differentiating this expression with respect to  $x$  again yields Eqn. ???.

$$\frac{d}{dx} \frac{4x^3}{e^x - e^{-x}} = \frac{12x^2}{e^x + e^{-x}} \quad (8)$$

In the limit that  $x$  approaches zero, the integrand also approaches zero; therefore, the expression for heat capacity overall also approaches zero. We insert this condition in our code using an if statement to set the output of the function for the heat capacity to zero at the lower limit of  $x=0$ .

### 3. RESULTS AND CONCLUSION

For Exercise 5.3, in part 'a', we develop the function to evaluate the integral of the given expression for a range of values for  $x$  from 0-3. To determine the appropriate number of slices to use, we plotted the approximation of the integral at a fixed value of  $x=2$  for various values of  $N$ . The logarithmic plot of the error is shown in Figure 1, where a precision on the order of  $10^{-3}$  is achieved for  $N \approx 10^{1.8} \approx 63$ .

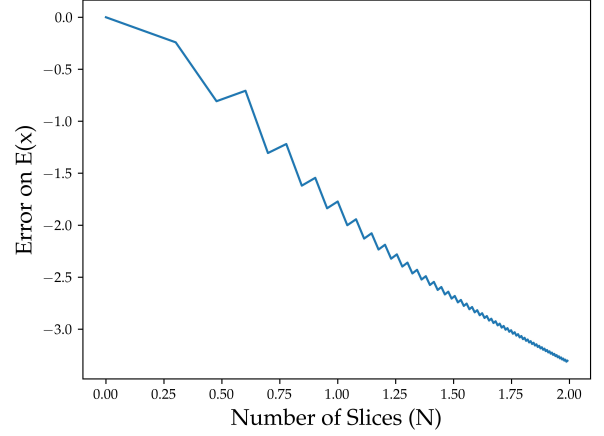


FIG. 1: A plot of the error on the integral approximation for the fixed upper limit of  $x=2$ . The chosen number of slices is  $N \approx 63$  to achieve a precision on the order of 0.001

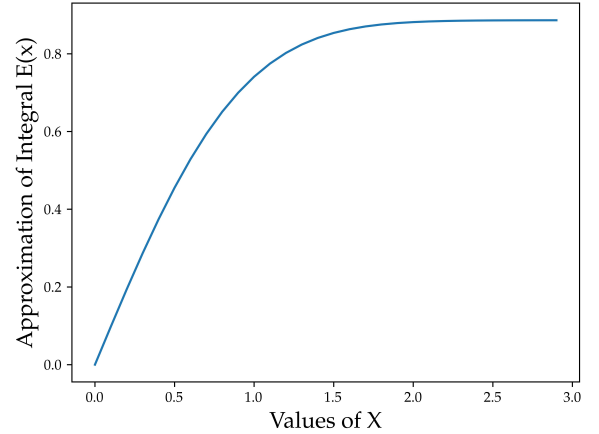


FIG. 2: A plot of the integral approximation for the range of values of  $x$  from 0-3.

Plotting the integral of the function in Eqn. 1 for multiple values of  $x$  from 0-3 with  $N$  fixed at a value of 63 slices, we obtain the plot shown in Figure 2.

For Exercise 5.9, we define the function to determine the heat capacity and run it for a range of temperatures from 5-500K. An example of the output heat capacity for an input temperature equal to that of the Debye temperature (428K) is 2111.6 J/K. The dependence of the heat capacity on temperature is shown in Figure 3.

We observe that at low temperatures, the heat capacity approaches zero, as noted by the proportionality to  $T^3$ . Einstein's model of heat capacity describes this relationship as the impact of a lower limit of the energy

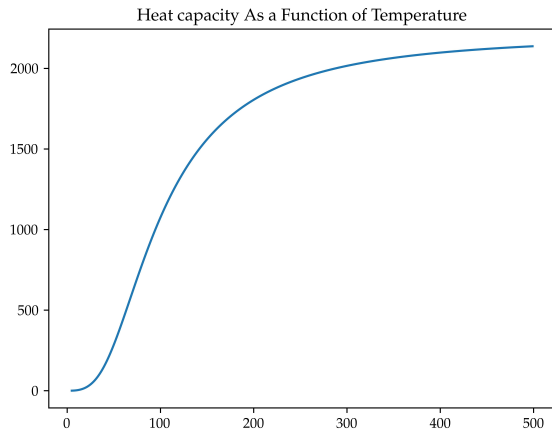


FIG. 3: A plot of the heat capacity for a sample of aluminum as a function of temperature.

possessed by atoms of solid matter that cannot go below the ground state energy, enforcing a “zero limit temperature” [2]. As  $T$  increases, we observe that the heat capacity approaches a constant value. This is

described in terms of Debye’s model, that compares atoms in a solid state to quantized packets of sound waves, or phonons, that oscillate at particular normal modes. According to [2], as the temperature increases, the frequency of oscillations increases as well. However, there exists a maximum mode of oscillation for these phonons beyond which the frequency cannot increase. The flattening out of the curve represents the approach of the heat capacity to this characteristic frequency, known as the Debye frequency, beyond which increasing temperature cannot further increase the heat/oscillations of the system. For further description, see the codes attached in the folders. The outputs are printed in each code file.

#### 4. SURVEY QUESTION

The most interesting problem was 5.9. The homework took me about 7 hours to complete. I learnt how to apply the coding we have been learning to practical concepts in Physics, particularly in quantum mechanics, and apply numerical integration. I think the problem set length and difficulty were just right.

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- [1] M. Newman, *Computational Physics* ([Createspace], 2012), URL <http://www-personal.umich.edu/~mejncp/index.html>.  
 [2] *Solid state heat capacity debye model: Quantum*

*tinkerer*, URL [https://solidstate.quantumtinkerer.tudelft.nl/2\\_debye\\_model/](https://solidstate.quantumtinkerer.tudelft.nl/2_debye_model/).