Homework 4 Part 2: Calculating the Heat Capacity of Aluminum

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An algorithm was written to calculate and graph the heat capacity of 1000cm^3 of solid aluminum with respect to temperature.

1. INTRODUCTION

The heat capacity of a solid material at constant volume is given by the equation:

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

where V is the volume of the material, θ_D is the Debye temperature of the material and ρ is the number density of atoms.[1] This equation for the heat capacity is derived from Debye's theory of solids.[1] The Debye temperature depends on the density of the material as well as the speed of sound through the material.

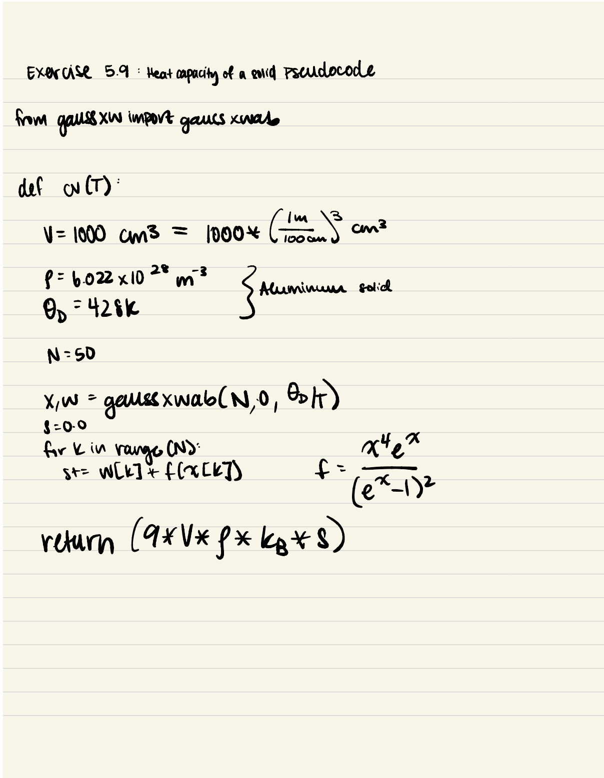

FIG. 1: Pseudocode for a general version of Simpson's rule including the approximation error calculation

2. EXPERIMENT

In this algorithm, we calculated the heat capacity for 1000cm^3 of solid aluminum, which has Debye temperature $\theta_D = 428$K and number density $\rho = 6.022 \times 10^{28}$m^{-3}. The integral in Eq. 1 was evaluated using Gaussian quadrature with $N = 50$ sample points. This function outlined in Fig. 1 was used to calculate and plot the heat capacity as a function of temperature from $T = 5$K to $T = 500$K.

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3. RESULTS

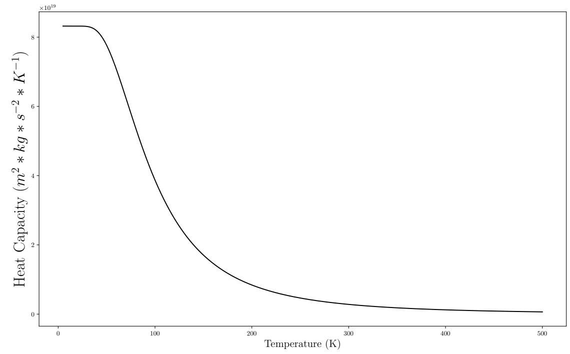

FIG. 2: Heat capacity of 1000cm^3 of Aluminum as a function of temperature.

As can be seen in Fig. 2, when the temperature is less than 50K, the heat capacity of aluminum is extremely high (on the order of 10^{20}) and relatively constant. Over the range of $T \approx 50$ to $T \approx 150$, the heat capacity decreases dramatically, then asymptotically approaching 0 for $T > 150$.

4. CONCLUSIONS

The Debye heat capacity decreases non-linearly with temperature, with a maximum of about 8.5×10^{19} at low temperatures and approaching zero at high temperatures.

[1] M. Newman, *Computational Physics* (2013), revised and expanded ed., ISBN 978-1-4801-4551-1.

Appendix A: Declaration of Collaborators

I did not collaborate with anyone on this assignment.

Appendix B: Survey Question

This assignment took me a much more reasonable amount of time, I was able to complete it in one day with 0.5 hours of writing pseudocode, 1 hour of coding, and 2 hours of writing the report. I thought it was cool to be able to do a calculation and visualize a graph of a subject that I have engaged with in 2 of my other physics classes in a new way. Last semester, I used this equation to describe properties of materials in Condensed Matter Physics, so it's neat to be engaging with the material in a new way.