Quantum Approach to Solids - Problem Sheet 3

Background: Increasingly the most of the most interesting results in physics are not solvable analytically. Thankfully at the same time, computing power has grown exponentially larger, and computer languages have become more intuitive and helpful to the coder. We need not only solve for the asymptotic limits of a function. Indeed, nowadays solving problems numerically is an important skill for even the most die-hard theoretical physicist.

Task: Using a numerical integration method of your choice[1], calculate the Debye heat capacity for a monatomic solid over a temperature range from 0 K to 300 K, using Debye temperatures of 50 K and 750 K.

Plot both of your results on the same graph, making sure that the axes are labelled, and that there is a legend. Your temperature axis should stop at 300 K. Include a dashed line across the full temperature range indicating the Dulong-Petit value of the heat capacity.[2] **[5]**

Reminder: the Debye heat capacity is given by:

$$C_V = 9Nk_B(\frac{T}{\Theta_D})^3 \int_0^{\frac{\Theta_D}{T}} \frac{x^4 \mathrm{e}^x}{(\mathrm{e}^x - 1)^2} \mathrm{d}x.$$

Note: Your work will only be assessed on the basis of the output obtained. However, you must include a copy of the code used, or other proof of method used, with your submission.

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[1] For example (but by no-means limited to) python, C, Maple, Mathematica, Wolfram Alpha online.

[2] **Extra**: (You are not expected to submit.) Now you have a working code, the interested might rerun it over the smaller temperature range of 0 to 50 K. Replot the data on this time with axes of C/T vs T^2, and confirm that the Debye model has the correct asymptotic limit as $T \to 0$.