Homework 2

Due Mar 19, 2024

Mar. 12, 2024

Problem 2.1

Exercise 5.9: Heat capacity of a solid

Debye's theory of solids gives the heat capacity of a solid at temperature T to be

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

where V is the volume of the solid, ρ is the number density of atoms, k_B is Boltzmann's constant, and θ_D is the so-called *Debye temperature*, a property of solids that depends on their density and speed of sound.

a) Write a Python function `cv(T)` that calculates C_V for a given value of the temperature, for a sample consisting of 1000 cubic centimeters of solid aluminum, which has a number density of $\rho = 6.022 \times 10^{28}\,\mathrm{m}^{-3}$ and a Debye temperature of $\theta_D = 428\,\mathrm{K}$. Use Gaussian quadrature to evaluate the integral, with $N = 50$ sample points.

b) Use your function to make a graph of the heat capacity as a function of temperature from $T = 5\,\mathrm{K}$ to $T = 500\,\mathrm{K}$.

Problem 2.2

Exercise 5.15: Create a user-defined function `f(x)` that returns the value $1 + \frac{1}{2}\tanh 2x$, then use a central difference to calculate the derivative of the function in the range $-2 \leq x \leq 2$. Calculate an analytic formula for the derivative and make a graph with your numerical result and the analytic answer on the same plot. It may help to plot the exact answer as lines and the numerical one as dots. (Hint: In Python the tanh function is found in the `math` package, and it's called simply `tanh`.)

Problem 2.3

Exercise 5.16: Even when we can find the value of $f(x)$ for any value of x the forward difference can still be more accurate than the central difference for sufficiently large h. For what values of h will the approximation error on the forward difference of Eq. (5.87) be smaller than on the central difference of Eq. (5.95)?