

Homework 7

Due Thursday, March 7th

Problem 1

(a) Write a computer program to compute the equation of state of a **relativistic** monatomic ideal gas. In practice, you can just make a plot of the energy E as a function of temperature for the gas.

Do this by computing the partition function $Z(\beta)$ by explicit numerical integral, and then taking the derivative of $\ln(Z)$ numerically (by sampling its value at neighboring points and measuring the slope). Show that you get the non-relativistic and ultra-relativistic limits correct and that it transitions at the right temperature.

(b) Take a derivative of $E(T)$ with respect to temperature to get the heat capacity (at constant volume) as a function of temperature. Plot the molar heat capacity as a function of temperature.

Make sure both of the regimes along with the transition point are clearly visible in your plots of $E(T)$ and $C_V(T)$.

Problem 2

Write a computer program to compute the equation of state of a nonrelativistic diatomic ideal gas. Again, just make a plot of $E(T)$. Treat the linear momentum integral classically, but include a full computation of the angular momentum term in quantum mechanics:

$$E(p, j) = \frac{p^2}{2m} + \frac{\hbar^2}{2I}j(j+1) \quad (1)$$

(the last term just being the eigenvalue of J^2). When performing the sum over quantum states, remember that there are $2j+1$ possible eigenstates for every value of j , so the sum looks like:

$$Z = \int \frac{d^3x d^3p}{h^3} \sum_{j=0}^{\infty} \sum_{m=-j}^j e^{-\beta E(p, j)} \quad (2)$$

Once you have $E(T)$, once again compute the heat capacity $C_V(T)$ (again using numerical derivative). Check behavior at low and high temperatures.

Problem 3

Compute the heat capacity per particle in a two-state system with energy separation ΔE . Make a plot of this heat capacity as a function of $\beta\Delta E$. Where is it comparable to the heat capacity you would estimate for a classical system like a gas?

Problem 4

Assuming I am technologically competent, I have attached a dataset to this assignment containing the molar heat capacity of diamond (in J/K) for a range of temperatures. Use this dataset to determine the characteristic vibrational frequency of carbon atoms in a diamond.

Are there parts of our theory of solids that predict the wrong answer?