

Homework #11

MSAE-E4201 Spring 2017

Due April 18 before 5:30 pm in course mailbox

1. (15 points) Molecules in a gas have translational energy $mv^2/2$.
 - (a) Use canonical ensemble methods to show that in one dimension, say the x direction so the energy per molecule is $mv_x^2/2$, the average energy per molecule is $k_B T/2$. (The partition function sum should be converted in an integral.)
 - (b) Use the result in part (a) and the factoring of partition functions to get the result for three dimensions, for which the molecules each have energy $(m/2)(v_x^2 + v_y^2 + v_z^2)$.
 - (c) Show that you get the same answer in 3D for molecule energy $mv^2/2$, where v is now the magnitude of the velocity (in spherical coordinates). (Now the integrating factor for this isotropic distribution in the partition function is $4\pi v^2 dv$ (instead of dv).)
 - (d) From this, obtain the specific heat per mole for each degree of freedom of translation.
2. (10 points)
 - (a) The rotational energy levels of a diatomic molecule are at $BJ(J+1)$, where $J = 0, 1, 2, 3, 4, \dots$. The degeneracy of each level is $2J+1$. Find the partition function in the high-T limit by converting the sum into an integral, and from this obtain the specific heat (per mole).
 - (b) In class we said that each rotational degree of freedom has a specific heat of $R/2$ in the high-temperature limit. Does or does not your result in (a) agree with this, and why is this so?
3. (40 points)
 - (a) The calculation in problem 1 leads to the correct specific heat, but needs to be more complete to calculate other quantities. It is helpful to first change velocity to momentum, so the corresponding kinetic energy in 1D is $p_x^2/2m$ (and this does not change the results for that problem). Now, for each atom (or molecule), the classical partition function integral for each dimension needs to be over phase space (momentum space and real space), $dp_x dx$ for each degree of freedom (and not just momentum space dp_x). Also, since the fundamental “volume” in phase space is h (Planck’s constant) per dimension, this differential is really $dp_x dx/h$. Show that the partition function for an atom in an ideal gas is $z = \alpha VT^{3/2}$, where T is temperature and V is the volume, and find the constant α .
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 - (b) Find the overall partition function Z for N atoms of the same type, assuming for now that the atoms are distinguishable.
 - (c) Show that the specific heat is unchanged and find the pressure P --and see how it compares to the ideal gas law.
 - (d) Find the entropy using the expressions for U and F in terms of Z , and then show that twice the entropy of this gas of N atoms in volume V does not equal that of a gas of $2N$ atoms in volume of $2V$ (which it should). (This is Gibb’s paradox: that putting a divider in this latter gas appears to change the entropy, but it should not.)
 - (e) Redo (b), (c), and (d) now with the atoms being indistinguishable, as they indeed are (by adding a factor of $1/N!$ in the overall partition function), and show there is no longer a Gibb’s paradox.
 - (f) A gas of N “A” atoms in volume V on the left side of a partition is allowed to expand into a volume $2V$ by removing the partition. At the same time a gas of N “B” atoms in volume V , which was initially the right side of this partition, is allowed to expand into this volume $2V$. Use

the results of (e) to find the increase in entropy, which is the entropy of mixing (and which is zero when all the atoms are of the same type).

4. (15 points) For non-interacting fermions at room temperature, calculate the probability that a state is occupied if its energy is: (a) 1 eV less than μ ; (b) 0.01 eV less than μ ; (c) equal to μ ; and (d) 0.01 eV greater than μ ; (e) 1 eV greater than μ . Sketch all on one plot vs. E for a given μ .

5. (20 points) For non-interacting bosons at room temperature, calculate the population (occupancy) of a state and the probabilities that the states with 0, 1, 2, or 3 bosons are occupied if its energy is: (a) 0.001 eV greater than μ ; (b) 0.01 eV greater than μ ; (c) 0.1 eV greater than μ ; and (d) 1 eV greater than μ . Sketch (a)-(d) for each on five plots vs. E for a given μ .